Electronic Supplementary Information

A Molecular Electron Density Theory Study of the Insertion of CO in Frustrated Lewis Pair Boron-Amidines: a [4+1] Cycloaddition Reaction

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1. Study of the structural characteristics of the frustrated Lewis pair (FLP) boron-amidine 4 in the equilibrium with the four-membered diazaborolone (4DAB) 2

In order to understand the role of the structural characteristics of FLP boron-amidine **4** in the equilibrium with the 4DAB **2**, the four equilibria given in Scheme S1 were analysed. 4DAB **2** is a strained four-membered species resulting from the formation of the new B1–N4 single bond, in which the N4 nitrogen and B1 boron centers become tetravalent. This compound is found −7.5 kcal·mol^{-1} below FLP boron-amidine **4**, in complete agreement with the experimental outcomes giving 4DAB **2** as the sole product in the absence of the CO molecule. However, this result contrasts with the usual displacement of the equilibrium towards the open form in the case of strained four-membered cycles. Therefore, it appears that the substituents present in FLP boron-amidine **4**, as well as the internal structure of the core framework itself, have a favourable stabilising effect which should overcome the unfavourable strain associated with the formation of 4DAB **2**.
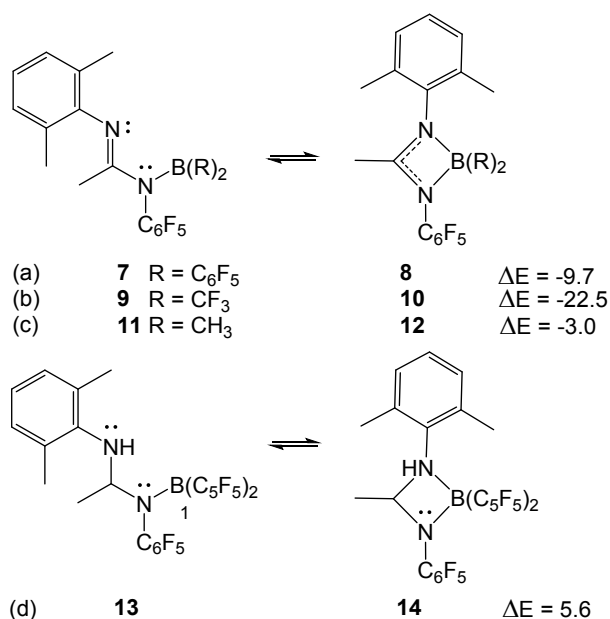
Scheme S1. Selected equilibria models for the study of the favourable formation of cyclic 4DAB **2**.

The substitution of the two isopropyl groups present in FLP boron-amidine **4** by two methyl groups in FLP boron-amidine **7** does not practically modify the equilibrium with 4DAB **8** (see Scheme S1).

When the two electron-withdrawing (EW) $-C_6F_5$ groups present in the B1 boron of FLP boron-amidine **7** are substituted by a stronger EW $-CF_3$ group, 4DAB **10** becomes 22.5 kcal·mol^{-1} more stable than FLP boron-amidine **9**. This result emphasizes the role of the EW substitution at the B1 boron in the stabilisation of the corresponding closed structure. However, it is noteworthy that a strong stabilisation of this closed species could be an unfavourable factor for the subsequent insertion of the CO molecule, which demands the aperture of this species. On the other hand, when the two EW $-C_6F_5$ groups present in the B1 boron of FLP boron-amidine **7** are substituted by an electron-releasing (ER) $-CH_3$ group, 4DAB **12** becomes only 3.0 kcal·mol^{-1} more stable than boron-amidine FLP **11**. This decrease of the stabilisation with ER groups also remarks the favourable role of the EW substitution at the B1 boron in the stabilisation of the corresponding closed structure.

Finally, when the C3–N4 double bond belonging to the N2–C3–N4 amidine framework of FLP boron-amidine **7** is hydrogenated to a diamine substructure as in FLP boron-amine **13**, the corresponding closed species **14** is found 5.6 kcal·mol^{-1} less stable than FLP boron-amine **13** (see equilibrium (d) in Scheme S1). Consequently, the presence of the N2–C3–N4 amidine framework also appears to have a significant role in the stabilization of 4DAB **2**. On the other hand, the substitution at N2 and N4 had no significant effects.

In summary, both the presence of EW groups at the tetrahedral B1 boron, as well as the presence of the N2–C3–N4 amidine framework, are the key factors stabilising the cyclic 4DAB **2** versus the open structure of FLP boron-amine **4**.

Table S1. ωB97X-D total, E, and relative, ΔE, electronic energies, in gas phase and in toluene, of the stationary points involved in the studied reaction paths associated with the domino conversion of hydrogenated boron-amidine **1** into 5DAB **3**. Total energies are given in atomic units, a.u., while relative energies are given in kcal·mol^{-1}. Relative energies for the dehydrogenation step are relative to **1**, while those for the carbonylation step are relative to **2** + CO.

	Gas phase		*Toluene*	
	E	ΔE	E	ΔE
H$_2$	-1.176071		-1.176144	
CO	-113.305480		-113.305813	
1	-2864.482028		-2864.488263	
TS-1	-2864.430791	32.2	-2864.435056	33.4
4	-2863.268275	23.6	-2863.272646	24.8
TS-2	-2863.259010	29.5	-2863.263015	30.8
2	-2863.279739	16.5	-2863.284521	17.3
Path A				
TS-3	-2976.574424	6.8	-2976.578419	7.5
3	-2976.619382	-21.4	-2976.625987	-22.4
Path B				
TS-4	-2976.560263	15.7	-2976.564545	16.2
IN-1	-2976.567397	11.2	-2976.572152	11.4
[TS-5]	-2976.551233	21.3	-2976.555925	21.6
Path C				
TS-6	-2976.555326	18.8	-2976.559526	19.3
IN-2	-2976.563618	13.6	-2976.568192	13.9
TS-7	-2976.510864	46.7	-2976.515123	47.2
IN-3	-2976.544182	25.8	-2976.549363	25.7
[TS-8]	-2976.543699	26.1	-2976.548903	26.0

Table S2. ωB97X-D enthalpies, H, entropies, S, and Gibbs free energies, G, in atomic units, a.u., as well as the relative ones, ΔH and ΔG in kcal·mol^{-1}, and ΔS in cal·mol^{-1}·K^{-1}, computed at 105 ºC and 2 bar in toluene, of the stationary points involved in the studied reaction paths associated with the domino conversion of hydrogenated boron-amidine **1** into 5DAB **3**. Relative thermodynamic data for the dehydrogenation step are relative to **1**, while those for the carbonylation step are relative to **2** + CO.

	H	ΔH	S	ΔS	G	ΔG
H$_2$	-1.161847		31.446		-1.180797	
CO	-113.296477		47.499		-113.325101	
1	-2863.917698		310.335		-2864.104716	
TS-1	-2863.871528	29.0	311.332	1.0	-2864.059146	28.6
4	-2862.725459	19.1	311.680	32.8	-2862.913286	6.7
TS-2	-2862.717383	24.1	301.309	22.4	-2862.898961	15.7
2	-2862.737428	11.6	303.998	25.1	-2862.920626	2.1
Path A						
TS-3	-2976.021324	7.9	320.414	-31.1	-2976.214414	19.6
3	-2976.066356	-20.4	318.317	-33.2	-2976.258185	-7.8
Path B						
TS-4	-2976.008198	16.1	318.591	-32.9	-2976.200189	28.6
IN-1	-2976.013462	12.8	313.699	-37.8	-2976.202506	27.1
[TS-5]	-2975.998156	22.4	321.154	-30.3	-2976.191693	33.9
Path C						
TS-6	-2976.002890	19.5	319.042	-32.5	-2976.195153	31.7
IN-2	-2976.009615	15.2	317.126	-34.4	-2976.200725	28.2
TS-7	-2975.958411	47.4	311.683	-39.8	-2976.146240	62.4
IN-3	-2975.990394	27.3	319.256	-32.2	-2976.182787	39.5
[TS-8]	-2975.991382	26.7	315.823	-35.7	-2976.181707	40.2
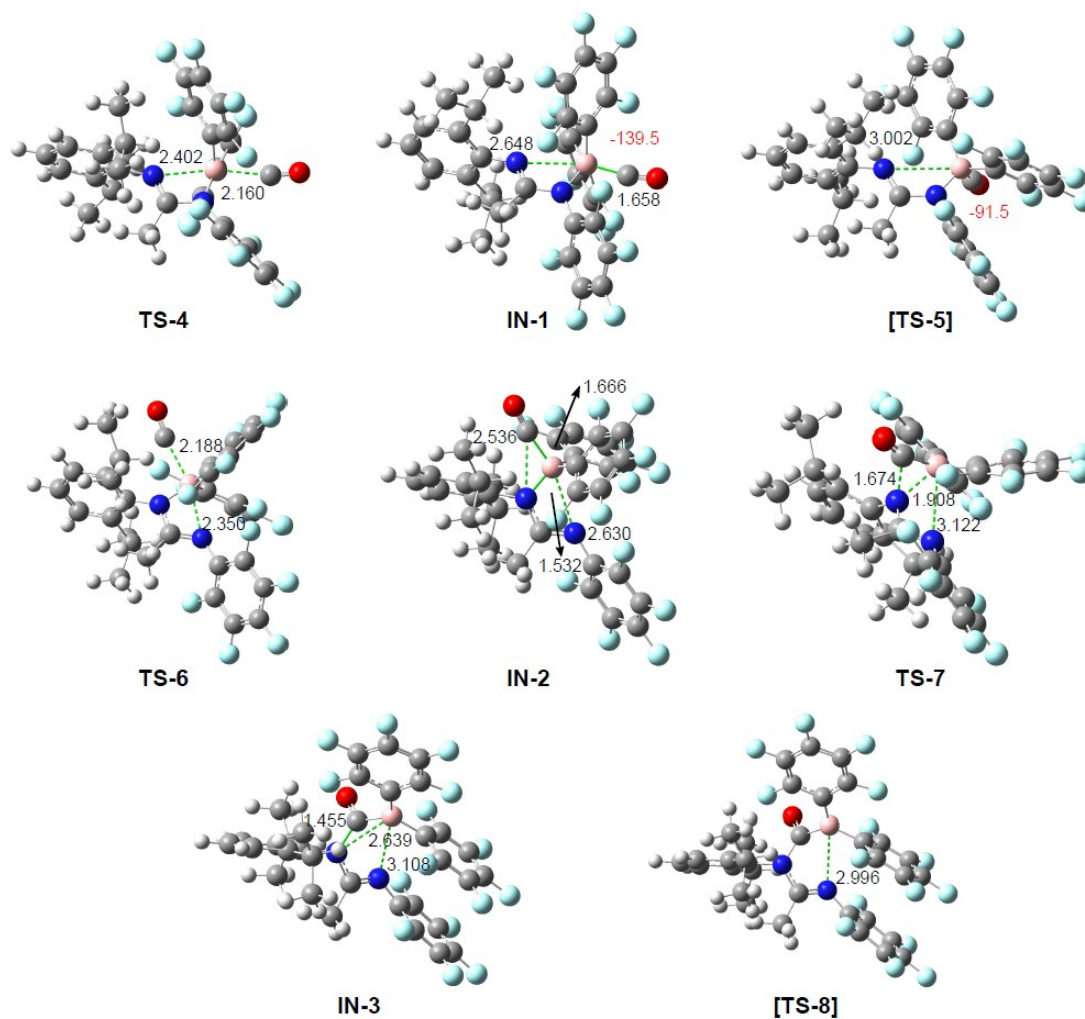
Figure S1. ωB97X-D gas phase geometries of the stationary points involved in the carbonylation of 4DAB **2** yielding 4DAB **3** along the unfavourable reaction paths B and C. Distances are given in angstroms, Å. The C5−B1−N2−C3 dihedral angle in **IN-1** and [**TS-5**], in sexagesimal degrees, º, is given in red colour.
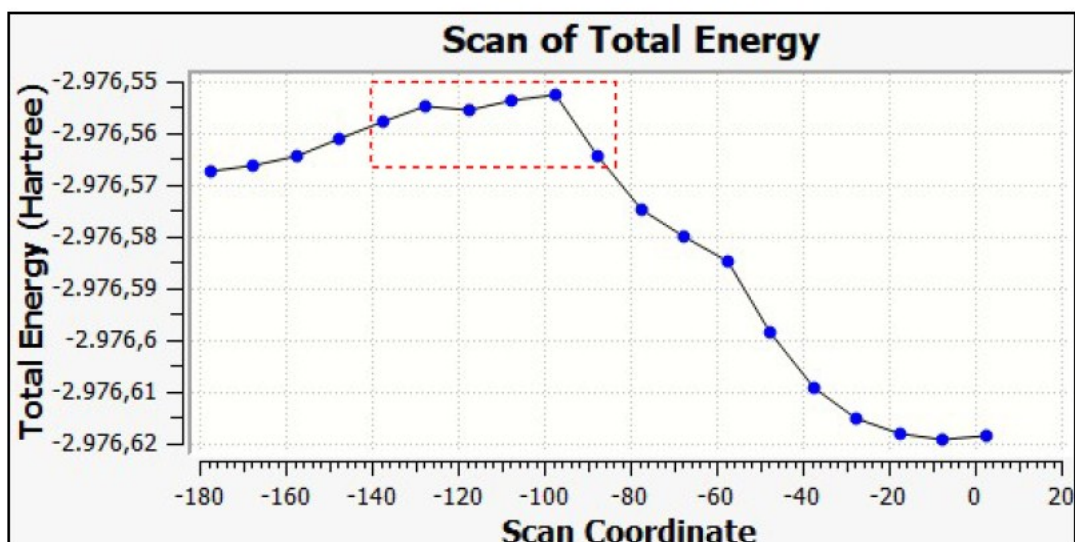
a)
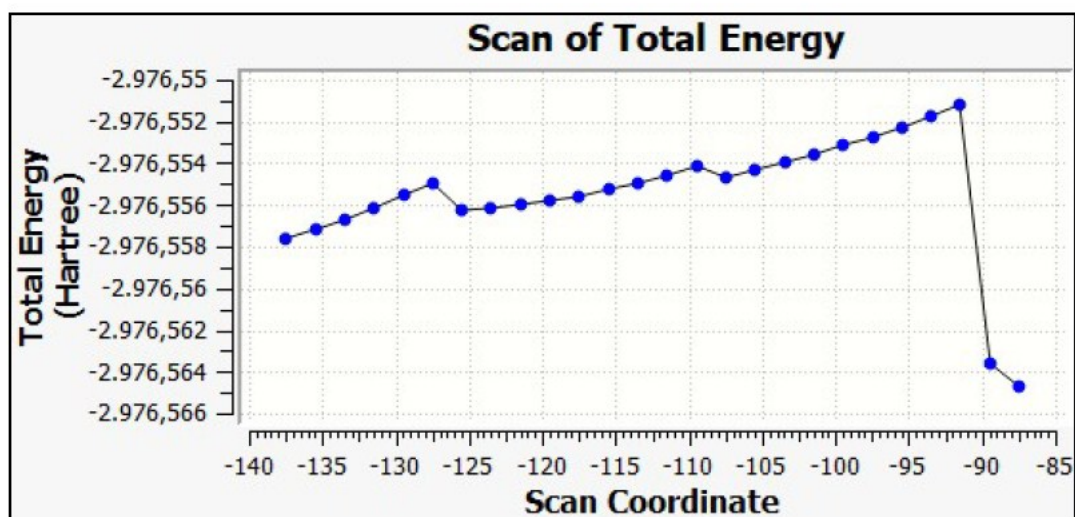
b)

Figure S2. Scan calculation from **IN-1** towards 5DAB **3** along the rotation of the C5–B1–N2–C3 dihedral angle by a) 10 degrees and b) 2 degrees for the angle range inside the red box of Figure a). The electronic energy of the maximum point of the scan profile b) was taken as an approximation to the electronic energy of [**TS-5**].
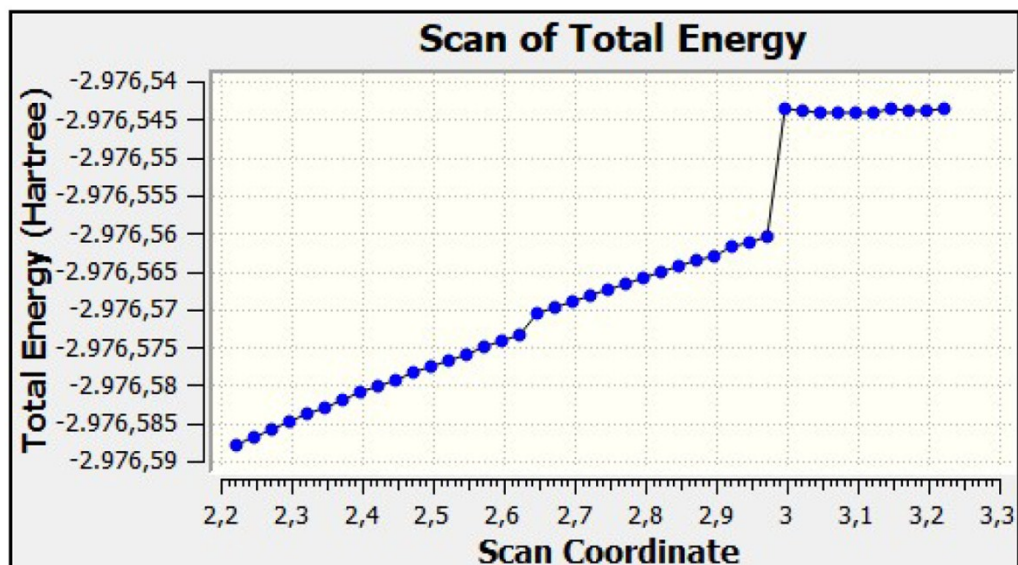
Figure S3. Scan calculation along the ring-closure step from **IN-3** towards 5DAB **3** decreasing the B1–N2 distance by 0.05 Å. The electronic energy of the maximum point of the scan profile was taken as an approximation to the electronic energy of [**TS-8**].

Table S3. ELF valence basin populations and distances of the forming bonds of the stationary points and the IRC structures involved in the formation of the new bonds along the most favourable reaction path A associated with the carbonylation reaction of simplified FLP boron-amidine **5** towards 5DAB **6**. The IRC values from **TS-9** to **6**, as well as the ELF analysis of **TS-3**, are also included. Electron populations are given in average number of electrons, e, distances in angstroms, Å, and RC values in atomic units, a.u.

	5	**CO**	**TS-9**	**S1**	**S2**	**S3**	**S4**	**6**	**TS-3**
IRC			0.000	3.627	3.696	18.985	19.054	34.273	
B1–C5			2.405	1.842	1.833	1.635	1.635	1.619	2.299
N4–C5			2.853	2.647	2.643	1.854	1.847	1.472	2.642
V(B1,N2)	4.06		2.64	2.32	2.31	2.09	2.09	3.35	3.98
V(N2)			1.53	1.86	1.86	2.00	2.00		
V(N2,C3)	1.80		1.76	1.76	1.76	1.86	1.87	2.47	1.99
V(C3,N4)	1.63		1.62	1.63	1.63	1.57	1.58	2.58	1.42
V'(C3,N4)	1.57		1.56	1.52	1.52	1.53	1.52		1.63
V(B1,N4)									
V(C5,O6)		3.23	3.30	1.89	1.89	1.43	1.43	2.49	3.27
V(C5,O6)				1.50	1.50	1.51	1.50		
V(O6)		3.99	4.00	4.03	4.03	2.06	2.09	2.54	4.12
V'(O6)						2.58	2.56	2.59	
V(N4)	2.55		2.56	2.56	2.56	2.39		0.64	2.67
V'(N4)								0.56	
V(C5)		2.58	2.48	2.46		0.08			2.51
V(B1,C5)					2.46	2.45	2.44	2.27	
V(N4,C5)							2.48	1.097	
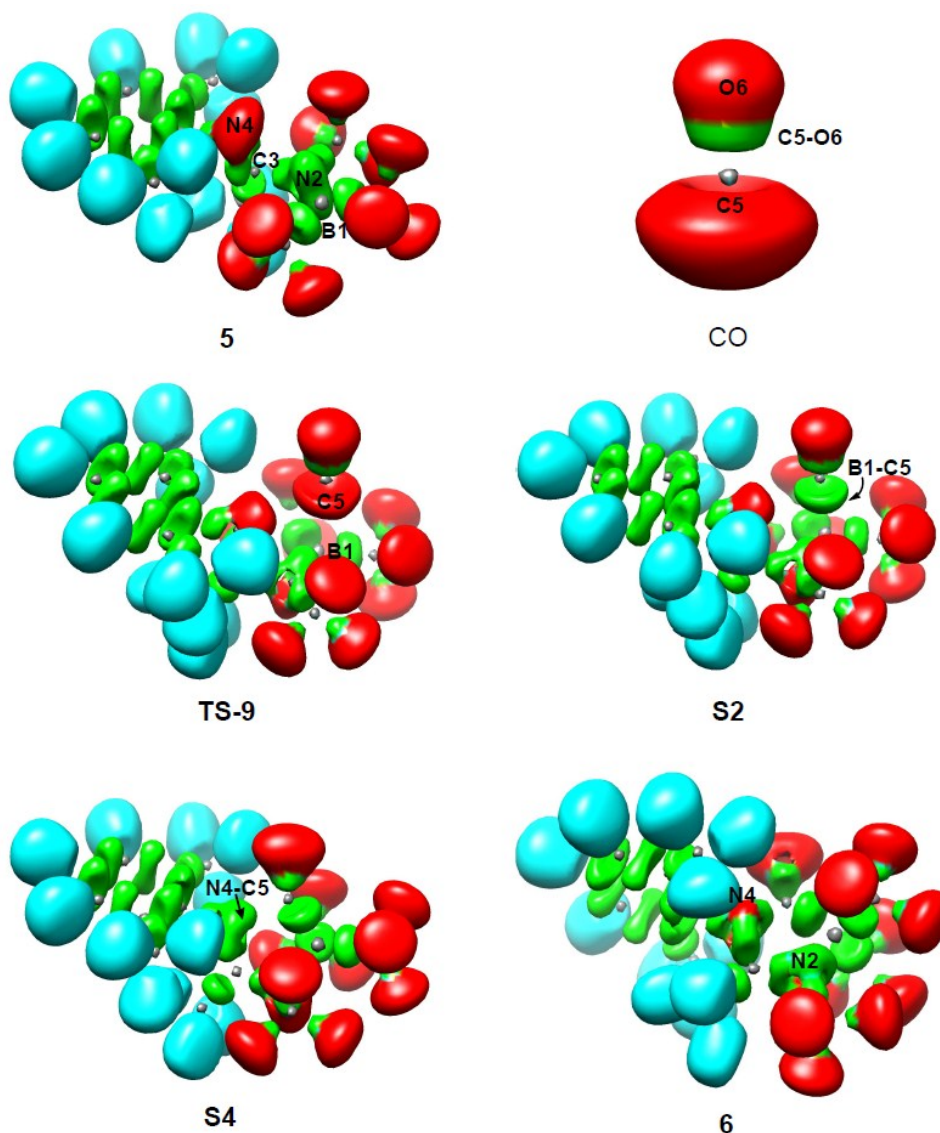
Figure S4. ELF localisation domains (isovalue = 0.75) for the stationary points and IRC structures involved in the formation of the two B1–C5 and N4–C5 single bonds the most favourable reaction path A associated with the carbonylation reaction of simplified FLP boron-amidine **5** towards 5DAB **6**. Monosynaptic valence basins are coloured in red, disynaptic valence basins in green, protonated basins in blue and core basins in grey.
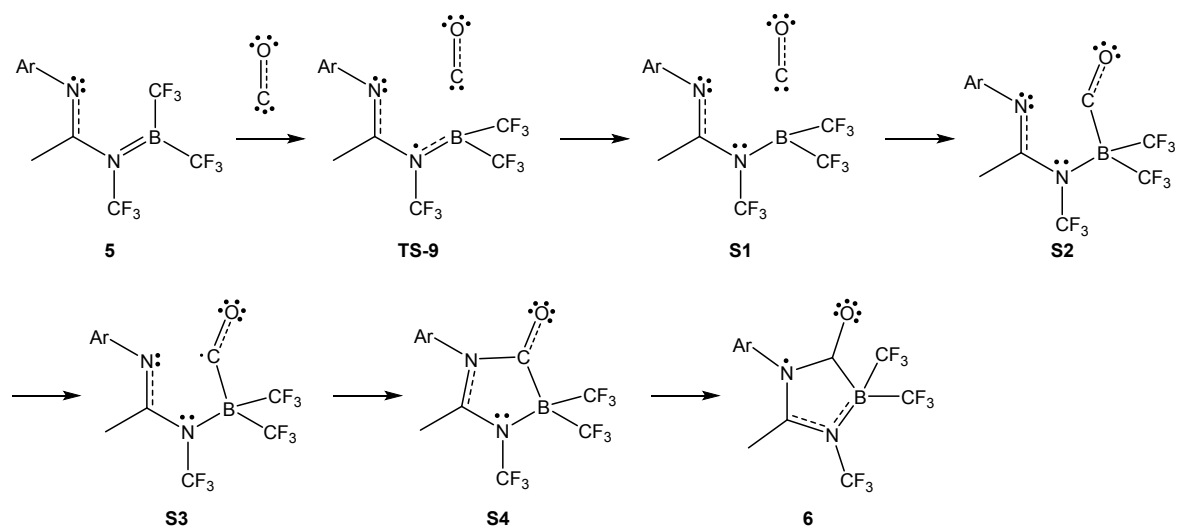
Scheme S2. Representation of the B1−C5 and N4−C5 bond formation processes along the most favourable reaction path associated with th carbonylation reaction of smaller FLP boron-amidine **5** towards 5DAB **6** by means of Lewis-like structures arising from the topological analysis of the ELF along the IRC. Ar = −C$_6$H$_3$(2,6-CH$_3$)$_2$

Cartesian coordinates of the stationary points involved in the studied reaction paths associated with the domino conversion of hydrogenated boron-amidine **1** into 5DAB **3**

1

E(RωB97X-D) = -2864.48202772 a.u.

C	3.30226700	-1.63719700	-0.27985500
C	3.35196800	-2.87529200	-0.93271300
C	4.58211300	-3.52911900	-0.97573000
C	5.70747600	-2.96814400	-0.39538400
C	5.63153000	-1.73541800	0.23638200
C	4.42712800	-1.04149500	0.30633900
H	4.66107200	-4.48697100	-1.47688600
H	6.65546700	-3.49212700	-0.44016300
H	6.52263300	-1.30893500	0.68010500
N	2.05455100	-0.92882600	-0.24035700
C	1.02713200	-1.25676200	0.53617700
N	-0.13113300	-0.65109700	0.34991800
B	-0.27461400	0.53495000	-0.72170900
C	1.24376500	-2.27771600	1.60556200
H	2.26012200	-2.19713800	1.98890900
H	0.53372600	-2.13411200	2.41744400
H	1.11381900	-3.28086900	1.19386500
C	2.14393000	-3.47496800	-1.63336500
H	1.24863300	-2.93396100	-1.32332000
C	4.33843100	0.33724200	0.93592600
H	3.33328100	0.45024100	1.34748500
H	1.84980800	-0.27886000	-0.99097600
H	0.19474600	0.09452400	-1.75565300
C	0.61672600	1.82940900	-0.29018900
C	1.22120400	2.07505700	0.93298000
C	0.84530100	2.80008500	-1.26010700
C	2.01177100	3.18567200	1.18336600
C	1.61654200	3.93063600	-1.05024600
C	2.21068600	4.12166300	0.18656300
C	-1.84574600	0.82504200	-0.98610300
C	-2.59890500	-0.13369600	-1.65427900
C	-2.54365600	1.95866900	-0.59209900
C	-3.95369900	-0.00778000	-1.90506500
C	-3.90031800	2.13110200	-0.83318700
C	-4.60895200	1.14154700	-1.49178200
C	-1.28260500	-1.14916900	1.00117500
C	-2.04515700	-0.34355100	1.84119200
C	-1.77047200	-2.41827400	0.70118800
C	-3.25895300	-0.78007000	2.34730900
C	-2.97003300	-2.87660300	1.21584900
C	-3.72090000	-2.04969100	2.03662900
F	0.29373600	2.65952900	-2.47144700
F	1.80170300	4.82323800	-2.01880400
F	2.99236500	5.17468100	0.40277300

F	2.62487600	3.32819100	2.35959300
F	1.11142900	1.20531300	1.95698400
F	-1.93418000	2.94883100	0.06722100
F	-4.52579000	3.23415400	-0.43156200
F	-5.90822100	1.28867500	-1.72280300
F	-4.62873900	-0.96921700	-2.53158900
F	-2.01260400	-1.27256700	-2.05701700
F	-1.07460300	-3.22413600	-0.09930200
F	-3.40525000	-4.09400300	0.92150700
F	-4.87247500	-2.47540000	2.53038700
F	-3.97575400	0.00979000	3.13364300
F	-1.63609600	0.87807100	2.14363800
C	5.32216800	0.55379200	2.08669300
H	6.35613900	0.61528000	1.73461100
H	5.09202200	1.49728000	2.58645700
H	5.25961500	-0.24758200	2.82723900
C	4.53103400	1.41138000	-0.14547300
H	5.48676000	1.26959700	-0.65811700
H	3.73560800	1.38217800	-0.89560100
H	4.53178200	2.40735000	0.30300700
C	1.92245900	-4.94718600	-1.27427900
H	2.72213700	-5.58530600	-1.66018000
H	1.87229100	-5.09418200	-0.19191400
H	0.98300800	-5.29866200	-1.70722300
C	2.26947600	-3.28505300	-3.15065400
H	2.37367800	-2.22793700	-3.40724300
H	3.14502200	-3.81386900	-3.53883900
H	1.38194400	-3.67226800	-3.65729900

TS-1
E(RωB97XD) = -2864.43079087 a.u.
Single imaginary frequency = -210.1751 cm^{-1}

H	-0.73743600	0.26087700	-1.48372500
H	-0.17572000	-0.11895400	-1.88669900
N	-1.84369700	1.06966500	-0.24581200
C	-0.93183000	1.34286400	0.60164600
N	0.24425100	0.59144000	0.50055600
B	0.27540800	-0.60469300	-0.36514800
C	-3.05557100	1.79517100	-0.32832400
C	-3.06658500	3.06828100	-0.92725400
C	-4.29163300	3.71894000	-1.05008900
C	-5.46672900	3.13327000	-0.60309300
C	-5.43750100	1.86825000	-0.03831700
C	-4.23879800	1.17459200	0.09807600
H	-4.33292300	4.70050200	-1.50664300
H	-6.40836200	3.66010100	-0.70705600
H	-6.36181200	1.41042300	0.29455700
C	-0.99464800	2.38812600	1.67639400
H	-1.99166400	2.82328800	1.71717000
H	-0.75391900	1.93413900	2.64003600

H	-0.27292300	3.18706600	1.48788200
C	-1.79408400	3.66903000	-1.50647000
H	-0.95214900	3.36739100	-0.87905500
C	-4.17448100	-0.20481900	0.72302400
H	-3.30613200	-0.69566500	0.27840300
C	1.73358200	-1.07832700	-0.83754000
C	2.32077500	-0.82393200	-2.06847900
C	2.50245000	-1.79926000	0.06725000
C	3.60123600	-1.25019500	-2.38787900
C	3.78646100	-2.23422700	-0.20945400
C	4.33699300	-1.95804800	-1.45170800
C	-0.79992900	-1.76174400	-0.11930400
C	-1.27457400	-2.53510700	-1.16998200
C	-1.29223900	-2.07768400	1.14057400
C	-2.22466300	-3.52918600	-1.01062900
C	-2.22416800	-3.08340100	1.34335800
C	-2.70425100	-3.80023200	0.26084500
C	1.45638900	1.18484800	0.92966500
C	1.97683400	0.95156400	2.19730800
C	2.18478400	1.99568400	0.06433600
C	3.19671700	1.48931500	2.58045900
C	3.40677000	2.53355600	0.42593400
C	3.91306300	2.27592200	1.69209300
C	-1.78914100	5.19801700	-1.53842000
H	-2.50615500	5.59217100	-2.26416500
H	-2.02827000	5.62195200	-0.55954900
H	-0.80085800	5.55900700	-1.83477500
C	-1.53761700	3.09493400	-2.90683200
H	-0.59288700	3.46826300	-3.31191500
H	-1.49165500	2.00414900	-2.88600400
H	-2.34300300	3.38362900	-3.58866500
C	-5.39248700	-1.08018400	0.42696600
H	-6.29148100	-0.71922900	0.93510200
H	-5.59997000	-1.12446600	-0.64500700
H	-5.21111900	-2.09921300	0.78096600
C	-3.93298700	-0.09639200	2.23419500
H	-3.01310700	0.45073800	2.45296800
H	-4.76247500	0.43208400	2.71399700
H	-3.84987700	-1.08482400	2.69241700
F	-0.82285400	-2.31017800	-2.41087500
F	-2.67128900	-4.22210500	-2.05175700
F	-3.62383500	-4.73819800	0.44057800
F	-2.68974700	-3.34200400	2.56241000
F	-0.90448900	-1.39428300	2.21762200
F	1.65979200	-0.14157600	-3.00933900
F	4.12543200	-0.98453900	-3.57790700
F	5.56324600	-2.36720200	-1.74039300
F	4.48941000	-2.90593700	0.69426300
F	2.00451900	-2.06903400	1.27968200
F	1.70103900	2.24844800	-1.14959600

F	4.09062100	3.29089700	-0.42126800
F	5.07838200	2.78889400	2.05337400
F	3.67916100	1.25772800	3.79344900
F	1.30396100	0.21848100	3.07000100

FLP boron-amidine **4**
E(RwB97XD) = -2863.26827486 a.u.

C	-3.08834600	1.67190800	-0.28164100
C	-3.21991000	2.98858500	-0.75818600
C	-4.45798000	3.61103400	-0.63575000
C	-5.54540400	2.94862300	-0.08622500
C	-5.41053400	1.63089200	0.31619800
C	-4.19174800	0.96357100	0.21240300
H	-4.57695600	4.63065100	-0.98443600
H	-6.50069700	3.45208400	0.00700800
H	-6.27040000	1.10487200	0.71681100
N	-1.81362100	1.05331100	-0.39772300
C	-0.99262900	1.09908500	0.55620400
N	0.30855500	0.50966300	0.33373000
B	0.51370100	-0.81492400	-0.08828100
C	-1.18797600	1.67783100	1.92866300
H	-2.17129400	2.13579600	2.01906200
H	-1.08616800	0.87390800	2.66272500
H	-0.42589600	2.42603400	2.15679000
C	-2.03811500	3.70806900	-1.38592600
H	-1.34261300	2.93950800	-1.72802100
C	-4.08063000	-0.49263500	0.62247800
H	-3.11656200	-0.84956500	0.26041500
C	-0.66084700	-1.86260100	-0.10650500
C	-1.18969400	-2.37546900	1.06629000
C	-1.16096800	-2.35897800	-1.29814000
C	-2.16527400	-3.35731900	1.06687400
C	-2.16293000	-3.31372600	-1.33731800
C	-2.65740700	-3.81836600	-0.14366200
C	1.96957200	-1.29497800	-0.46857600
C	2.57193900	-2.36038400	0.18764600
C	2.69582900	-0.70406000	-1.49444200
C	3.84077100	-2.81152700	-0.13655300
C	3.96374600	-1.13129600	-1.85038700
C	4.53637000	-2.19124700	-1.16371600
C	1.41326600	1.34902400	0.64079800
C	2.20746000	1.08568100	1.75251900
C	1.73330800	2.44638400	-0.15084800
C	3.29170100	1.88529700	2.06938500
C	2.80315600	3.26860400	0.16555900
C	3.58502700	2.98391600	1.27446400
C	-1.30421600	4.57822400	-0.35756200
H	-1.96364200	5.36506900	0.02171500
H	-0.96647800	3.99045600	0.49937000
H	-0.42737300	5.05110900	-0.80821400

C	-2.42977800	4.54045500	-2.60992100
H	-2.99460900	3.94272300	-3.32892300
H	-3.03631800	5.40958300	-2.33821500
H	-1.53072900	4.91477500	-3.10663200
C	-4.10758400	-0.65019800	2.14696300
H	-3.29569300	-0.09420600	2.62074900
H	-5.05033000	-0.27580900	2.55713600
H	-4.01006400	-1.69963300	2.43515600
C	-5.15586000	-1.36089900	-0.03925100
H	-6.16026000	-1.09325000	0.30017000
H	-5.12734800	-1.25763400	-1.12666400
H	-5.00140500	-2.41442400	0.20872600
F	1.92706100	0.04567200	2.52904900
F	1.01788300	2.72027600	-1.23004300
F	3.08626100	4.31736900	-0.59412900
F	4.04056600	1.61612800	3.12980300
F	4.61328900	3.76049700	1.57514500
F	1.93027700	-2.97117200	1.18507200
F	2.16990400	0.31189000	-2.18135400
F	4.62987100	-0.54348600	-2.83650700
F	5.74928300	-2.61092100	-1.48787700
F	4.39461700	-3.82195500	0.52163700
F	-2.65082400	-3.74968100	-2.49182200
F	-3.62413900	-4.72584500	-0.15927700
F	-2.66197200	-3.82972400	2.20598300
F	-0.76932700	-1.90413900	2.24518700
F	-0.67542700	-1.89704800	-2.45157800

H_2

E(RωB97X-D) = -1.17607105342 a.u.

H	0.00000000	0.00000000	0.37216100
H	0.00000000	0.00000000	-0.37216100

TS-2

E(RωB97X-D) = -2863.25901044 a.u.

Single imaginary frequency = -55.3392 cm^{-1}

C	-2.27722900	2.11417900	0.38519000
C	-3.49510900	1.98748400	-0.29946800
C	-4.56911000	2.77762700	0.11455900
C	-4.44682900	3.66420100	1.16701300
C	-3.23802500	3.76926800	1.84348900
C	-2.14287800	2.99894000	1.47747800
H	-5.52043400	2.68918400	-0.39891800
H	-5.29267900	4.27139900	1.46870200
H	-3.15180400	4.46647100	2.66791100
N	-1.13639000	1.33913600	0.07816900
C	-0.46320200	1.44049500	-1.00564900
N	0.51215200	0.45397700	-1.04883100
B	0.15339200	-0.55565400	-0.02808600

C	-0.69610800	2.35593800	-2.16223800
H	-1.20499300	1.79315900	-2.94953400
H	-1.32545400	3.19213100	-1.86004400
H	0.23628500	2.73755900	-2.57323100
C	-3.71585300	0.98319700	-1.41837700
H	-2.76675700	0.48998500	-1.63179900
C	-0.82724000	3.06611100	2.23537100
H	-0.02433000	2.96377000	1.50288400
C	-1.10800700	-1.48163500	-0.23670700
C	-1.58311900	-1.83842100	-1.49362600
C	-1.78500200	-2.03199700	0.84698500
C	-2.64485600	-2.71030600	-1.67078300
C	-2.84705500	-2.90616000	0.70828100
C	-3.27523300	-3.25089100	-0.56429600
C	1.23357300	-0.90585300	1.06788000
C	1.51218300	-2.20981100	1.47290600
C	1.96280700	0.09543200	1.70466100
C	2.43240700	-2.50630100	2.46330500
C	2.87296600	-0.16158100	2.71482300
C	3.10966800	-1.47320200	3.09291000
F	-1.41267400	-1.71965300	2.09151000
F	-1.04259600	-1.32554100	-2.60390500
F	-3.46894800	-3.40016700	1.77253000
F	-4.31268600	-4.05930500	-0.72096200
F	-3.09186300	-2.99353500	-2.89076200
F	0.89797200	-3.24222900	0.89644900
F	1.79398300	1.37479800	1.36768400
F	3.51673200	0.83141000	3.31742600
F	3.98456200	-1.74017000	4.04831400
F	2.67233900	-3.76336200	2.81499900
C	1.79081300	0.59669500	-1.58878100
C	2.43484700	-0.52671400	-2.10823300
C	2.51594800	1.78817500	-1.56443000
C	3.72315000	-0.46711500	-2.60886700
C	3.79452500	1.87095400	-2.09128800
C	4.40360500	0.74087500	-2.61188600
F	1.98915900	2.88659200	-1.02328400
F	4.44759700	3.02535200	-2.07081000
F	5.63270100	0.81189500	-3.10219200
F	4.30423000	-1.55671800	-3.09180200
F	1.80516100	-1.70040300	-2.09793600
C	-4.70062100	-0.10329500	-0.96996500
H	-5.68938800	0.32171000	-0.77647100
H	-4.81199900	-0.86891400	-1.74304700
H	-4.35921200	-0.58194000	-0.04943000
C	-4.19595700	1.64539400	-2.71473000
H	-3.51813900	2.43912500	-3.03734600
H	-4.26307800	0.90410700	-3.51585700
H	-5.18763400	2.08897800	-2.58977100
C	-0.71807500	1.88119000	3.20646200

H	-0.84251900	0.92848600	2.68845200
H	0.25823400	1.88207200	3.70035500
H	-1.49042500	1.95042300	3.97861100
C	-0.60332900	4.38628600	2.97253800
H	-0.71880100	5.24488600	2.30579700
H	-1.29590200	4.50824200	3.81101900
H	0.40879300	4.41002600	3.38427100

2DAB **2**
E(RωB97X-D) = -2863.27973929 a.u.

C	-2.17058100	0.90525500	-1.63550700
C	-3.15453100	-0.03560600	-1.98970800
C	-4.42616600	0.44260800	-2.30262800
C	-4.72198000	1.79338000	-2.25045900
C	-3.73649200	2.70238600	-1.90272200
C	-2.44503000	2.28177500	-1.60212800
H	-5.20256500	-0.26189700	-2.57958400
H	-5.72277300	2.13897200	-2.48299000
H	-3.97151300	3.76008200	-1.86903500
N	-0.86678700	0.46918100	-1.25838600
C	0.02771300	-0.16992900	-1.98215000
N	0.83010200	-0.67150500	-1.02157000
B	-0.11492400	-0.00117200	0.07089900
C	0.04371600	-0.26947500	-3.45947000
H	-0.94534400	-0.01498300	-3.83738800
H	0.76428800	0.44488000	-3.85766200
H	0.32937900	-1.26831600	-3.78633600
C	-2.91598600	-1.53835600	-2.03345100
H	-1.89791900	-1.74512600	-1.69869100
C	-1.37701000	3.30095600	-1.25297600
H	-0.41877800	2.78966800	-1.29626000
C	-1.08267200	-0.99511300	0.89340600
C	-1.00225000	-2.37949200	0.89538500
C	-2.12794000	-0.45888200	1.63273000
C	-1.85756200	-3.18156500	1.63646200
C	-2.99687100	-1.21976800	2.39327200
C	-2.85318400	-2.59808800	2.39918200
C	0.68596500	1.15969000	0.87566000
C	0.67503000	1.32422800	2.25794400
C	1.48912600	2.07316300	0.19587700
C	1.33297700	2.35889900	2.90795400
C	2.15611500	3.12214700	0.80265200
C	2.07274200	3.26996500	2.17622900
F	-2.31231400	0.86882300	1.64245000
F	-0.09819300	-3.02397300	0.14351100
F	-3.97005000	-0.64975900	3.09672000
F	-3.68748000	-3.35404900	3.10164800
F	-1.74666800	-4.50710200	1.59408100
F	0.02340500	0.47302400	3.05254100
F	1.65062100	1.98550700	-1.13929500

F	2.87360700	3.97835200	0.08081900
F	2.70594300	4.26407400	2.78281400
F	1.26833200	2.47235100	4.23001500
C	2.14413100	-1.11184400	-0.96903400
C	2.63053200	-1.59032900	0.25487400
C	3.06805800	-1.06821200	-2.01350300
C	3.92696100	-2.04455800	0.41272400
C	4.36579900	-1.53348900	-1.87310600
C	4.80562800	-2.02473500	-0.65780000
F	2.73278200	-0.56398500	-3.20361700
F	5.19401800	-1.48324900	-2.90908500
F	6.04862500	-2.46304300	-0.51778300
F	4.32924000	-2.49458500	1.59298200
F	1.84111400	-1.60620300	1.32568400
C	-3.86192700	-2.27349800	-1.07571400
H	-4.89062300	-2.25368700	-1.44640200
H	-3.56473600	-3.32064400	-0.97293500
H	-3.85717100	-1.81300800	-0.08799200
C	-3.06705100	-2.10492600	-3.45155300
H	-2.38428100	-1.63441200	-4.16169400
H	-2.86563300	-3.17958100	-3.45017900
H	-4.08429700	-1.95757600	-3.82501300
C	-1.56279800	3.83864000	0.17039200
H	-1.54811000	3.03187300	0.90410500
H	-0.76310600	4.54357400	0.41705300
H	-2.51795200	4.36405000	0.26679000
C	-1.30756200	4.44382700	-2.27113200
H	-1.19426700	4.06117000	-3.28864800
H	-2.20189300	5.07298100	-2.24368500
H	-0.44951200	5.08413000	-2.04985200

CO
E(RωB97X-D) = -113.305480126 a.u.

C	0.00000000	0.00000000	-0.64287100
O	0.00000000	0.00000000	0.48215300

TS-3
E(RωB97X-D) = -2976.57442398 a.u.
Single imaginary frequency = -160.8963 cm^{-1}

C	3.20656800	-1.58389200	-0.21406400
C	3.33814400	-2.84561400	-0.81820000
C	4.59548100	-3.44690900	-0.83698200
C	5.69870800	-2.82588500	-0.28044000
C	5.55785500	-1.57112500	0.29359100
C	4.32567700	-0.92770100	0.33093800
H	4.70785500	-4.42209400	-1.29895000
H	6.66756700	-3.31143300	-0.29954000
H	6.42612600	-1.08313600	0.72019300
N	1.94732500	-0.93247900	-0.23071000

C	1.04791300	-1.23076700	0.61455500
N	-0.21392000	-0.61610000	0.45896600
B	-0.39700700	0.62795500	-0.27687700
C	1.20265900	-2.18207100	1.76784900
H	0.75402100	-3.15139000	1.53891400
H	2.26101700	-2.34129600	1.96772200
H	0.71876300	-1.77710300	2.65803400
C	2.16532000	-3.55869200	-1.47192100
H	1.27285400	-2.94804700	-1.33619800
C	4.20114900	0.48148500	0.87803400
H	3.20653900	0.57717400	1.31491400
C	0.51409000	-0.06145600	-2.27183900
O	1.02399500	-0.38586100	-3.21968600
C	0.60101700	1.84252900	-0.06135000
C	0.78938000	2.82369300	-1.02688000
C	1.19700100	2.08618300	1.16930700
C	1.54589300	3.96201400	-0.81427800
C	1.95524300	3.21574400	1.42346800
C	2.13333400	4.15688900	0.42500700
C	-1.88465800	0.96173500	-0.74392100
C	-2.54547900	2.11493800	-0.33308400
C	-2.62275000	0.09640700	-1.54526900
C	-3.85599900	2.39487100	-0.68860700
C	-3.92946300	0.34357500	-1.92569400
C	-4.54963100	1.50509500	-1.49154100
C	-1.34636400	-1.27691100	0.98801200
C	-1.73123200	-2.54318200	0.55716000
C	-2.14836800	-0.65032700	1.93848600
C	-2.86149500	-3.16841400	1.05516800
C	-3.29728600	-1.24818100	2.42776900
C	-3.65080700	-2.51481400	1.98912800
C	1.88969500	-4.91874900	-0.82021100
H	2.71352000	-5.61783000	-0.99204000
H	1.75811100	-4.82287200	0.26044000
H	0.98173300	-5.36385200	-1.23582500
C	2.38163700	-3.70769800	-2.98242400
H	2.55003000	-2.73601500	-3.45149500
H	3.24771700	-4.34045400	-3.19844100
H	1.50574000	-4.16715500	-3.44950400
C	5.20414500	0.81703400	1.98274100
H	4.94327800	1.77691100	2.43500600
H	5.20284600	0.05867500	2.76962500
H	6.22313400	0.90652200	1.59481000
C	4.31759900	1.48080000	-0.28168200
H	5.25927500	1.32714200	-0.81641800
H	3.49748100	1.35441200	-0.99308400
H	4.30758300	2.51010400	0.08592500
F	0.21384200	2.69102600	-2.22962100
F	1.06674700	1.21985600	2.18085200
F	2.54676000	3.38132400	2.60256000

F	2.88828600	5.22348200	0.64416400
F	1.71223700	4.86089700	-1.77702800
F	-1.94110400	3.00134600	0.45888800
F	-2.07200700	-1.04399200	-1.98136700
F	-4.58998500	-0.51506800	-2.69325500
F	-5.80114700	1.75856500	-1.83941200
F	-4.45010500	3.50260000	-0.26364200
F	-1.83147800	0.56412900	2.37299800
F	-4.05230300	-0.62097000	3.31930500
F	-4.74033200	-3.09978200	2.46128200
F	-3.19804600	-4.37992000	0.63397200
F	-0.99756600	-3.18401800	-0.34824600

5DAB **3**
E(RωB97X-D) = -2976.61938212 a.u.

C	2.91973000	1.88657200	-0.02771000
C	4.10371400	1.24952600	0.36803200
C	5.28479200	1.97873900	0.27083900
C	5.28036300	3.28246500	-0.20327700
C	4.09400500	3.88537900	-0.58678000
C	2.88385700	3.19936300	-0.50719200
H	6.22173700	1.52099500	0.56442100
H	6.21285800	3.83046500	-0.27744100
H	4.10733200	4.90153800	-0.96411800
N	1.69715700	1.13885800	0.02204500
C	0.82855700	1.16603700	1.03707800
N	-0.21555100	0.38026800	0.85607100
B	-0.08697700	-0.45202700	-0.48655300
C	1.07930300	1.99931200	2.23918600
H	2.11017900	1.84828400	2.56334600
H	0.95919700	3.05502500	1.98608500
H	0.39651000	1.73661000	3.04471000
C	4.10638000	-0.19214500	0.84623000
H	3.11225400	-0.41637900	1.23413700
C	1.59686400	3.85440200	-0.97475800
H	0.75675300	3.22620700	-0.67450200
C	1.17367700	0.36771300	-1.11293200
O	1.75294000	0.36891300	-2.15617200
C	0.58146400	-1.92181500	-0.25168200
C	1.23955700	-2.33100200	0.90002600
C	0.69890600	-2.78833700	-1.33420500
C	1.96107800	-3.51075500	0.98843100
C	1.39485300	-3.98379600	-1.28215700
C	2.03777600	-4.34665400	-0.10975600
C	-1.48201500	-0.34492800	-1.28369600
C	-2.44300400	-1.34531700	-1.33260400
C	-1.82801600	0.84599800	-1.90808800
C	-3.65652300	-1.19301400	-1.98640800
C	-3.02751200	1.04245700	-2.57002000
C	-3.94757700	0.00757000	-2.61270800

C	-1.40146500	0.49370500	1.60310800
C	-2.01851100	-0.61965200	2.16758700
C	-2.07719300	1.71160500	1.66838200
C	-3.25208200	-0.51298300	2.79188800
C	-3.29891300	1.83573100	2.30486100
C	-3.89027000	0.71486100	2.86699800
F	-1.54249300	2.79180000	1.09956900
F	-5.06098800	0.81768700	3.47358600
F	-3.81960000	-1.58389900	3.32490400
F	-1.44980900	-1.81119700	2.10335100
F	-3.90855800	3.01092600	2.36343600
F	-0.98557100	1.89175900	-1.86080800
F	-3.30609800	2.20576600	-3.15087500
F	-5.10587300	0.17072900	-3.23833700
F	-4.54501000	-2.18146200	-2.00816600
F	-2.23526600	-2.51663300	-0.72312900
F	0.12851500	-2.47520600	-2.50089200
F	1.46453600	-4.77707200	-2.34569800
F	2.73212700	-5.47610500	-0.04590000
F	2.60669600	-3.82315800	2.11135800
F	1.25541400	-1.56419600	2.00958000
C	5.08803000	-0.44790700	1.99247900
H	6.12837900	-0.39583600	1.65914600
H	4.95562600	0.27299100	2.80377100
H	4.92421100	-1.44978800	2.39662400
C	4.37431100	-1.14742500	-0.32599400
H	3.63299500	-1.03286000	-1.11875700
H	5.36010900	-0.95248000	-0.75869900
H	4.35473300	-2.18470600	0.02002200
C	1.38026200	5.23028000	-0.33725900
H	2.12701300	5.95495900	-0.67321800
H	0.39698000	5.61935100	-0.61281900
H	1.43341400	5.18061000	0.75435300
C	1.56841100	3.93134300	-2.50634900
H	2.37114500	4.57690700	-2.87599700
H	1.69510100	2.94012600	-2.94503300
H	0.61457800	4.34130600	-2.84784200

TS-4
E(RωB97X-D) = -2976.56026304 a.u.
Single imaginary frequency = -222.0745 cm^{-1}

C	1.80426000	1.31902800	-1.84755600
C	1.70320700	2.72188900	-1.86137500
C	2.62697100	3.44605400	-2.61270800
C	3.64211800	2.81322600	-3.30833900
C	3.75825000	1.43252200	-3.24549100
C	2.85575500	0.66504600	-2.51664000
H	2.54913600	4.52722500	-2.65128800
H	4.34961900	3.39408800	-3.88897200
H	4.56873300	0.94439000	-3.77406500

N	0.88457400	0.57473200	-1.07728700
C	-0.27510400	0.24825700	-1.49902600
N	-1.05416600	-0.36823500	-0.53217900
B	-0.23768700	-0.52930200	0.73724300
C	-0.79751600	0.38285500	-2.89832200
H	-1.15199700	-0.59013500	-3.24724400
H	-1.62457500	1.09074900	-2.95637200
H	0.00241700	0.72987700	-3.55061800
C	0.62053900	3.45931000	-1.08798500
H	0.15516200	2.74381800	-0.40661600
C	3.03728400	-0.83517700	-2.38073500
H	2.04908400	-1.27415400	-2.24573800
C	-1.72576300	-1.40067100	2.03886700
O	-2.25442300	-1.91338700	2.88400400
C	-0.03148200	0.79999800	1.60745400
C	-1.10402600	1.60727800	1.95923200
C	1.22824700	1.31834600	1.89231900
C	-0.96367200	2.85750000	2.53817900
C	1.41034700	2.56124000	2.47048200
C	0.30831200	3.33761300	2.79169800
C	0.72498900	-1.79603800	0.87472500
C	1.38076500	-2.08338900	2.06924500
C	0.99038600	-2.67391800	-0.17444000
C	2.29139400	-3.11423500	2.21307400
C	1.90169100	-3.71107000	-0.07073600
C	2.56320100	-3.92757800	1.12518300
C	-2.41841000	-0.61580900	-0.72178600
C	-3.31406800	0.42809700	-0.96117200
C	-2.95404100	-1.90089500	-0.64813800
C	-4.66519200	0.20483500	-1.15717300
C	-4.30952500	-2.14023100	-0.81008000
C	-5.16725400	-1.08537800	-1.07623100
C	-0.47073900	3.99260000	-2.02347800
H	-0.05913000	4.73732400	-2.71179600
H	-0.90843800	3.19378000	-2.62458600
H	-1.27424000	4.46562300	-1.45180900
C	1.19575300	4.59829000	-0.23757100
H	2.01546300	4.25079300	0.39489400
H	1.57886300	5.41170200	-0.86001700
H	0.41865200	5.02182800	0.40554100
C	3.65616700	-1.50567000	-3.60821600
H	3.12505000	-1.23474600	-4.52447800
H	4.70993300	-1.24009400	-3.73448900
H	3.60756000	-2.59185600	-3.49424400
C	3.86572700	-1.13613700	-1.12285600
H	3.36872700	-0.75941800	-0.22656100
H	4.02526500	-2.21293600	-1.01227600
H	4.84668600	-0.65660200	-1.19366200
F	0.40090000	-2.54292100	-1.36513000
F	2.16824100	-4.47885600	-1.12244900

F	3.44728900	-4.90720500	1.22849900
F	2.89562000	-3.33335700	3.37452400
F	1.11865300	-1.35592800	3.16207300
F	-2.86742800	1.68019300	-1.01375200
F	-2.16164900	-2.93737000	-0.38003100
F	-4.78460300	-3.37576700	-0.72155800
F	-6.46149700	-1.30700300	-1.24661600
F	-5.48426900	1.21906200	-1.39984500
F	2.32970800	0.64206100	1.57436500
F	2.63245000	3.03699600	2.68307600
F	0.47432200	4.54376700	3.31401100
F	-2.02847000	3.59296600	2.83952100
F	-2.36286800	1.18448800	1.73997700

IN-1

E(RωwB97X-D) = -2976.56739740 a.u.

C	-1.60284700	1.50443800	-1.85674800
C	-2.65466900	0.94723000	-2.60742200
C	-3.43390600	1.79374100	-3.38931200
C	-3.19743900	3.16000500	-3.42748800
C	-2.18363900	3.69871600	-2.65441300
C	-1.38063600	2.89302700	-1.84965800
H	-4.24204300	1.37927200	-3.98066900
H	-3.81140800	3.80213300	-4.04856800
H	-2.01166000	4.76962500	-2.67285300
N	-0.81120700	0.68852400	-1.02206500
C	0.30933900	0.21728100	-1.39440900
N	1.03809600	-0.48449600	-0.43163800
B	0.33940100	-0.71432200	0.90717200
C	0.87154500	0.27519400	-2.78968600
H	0.11489000	0.66792800	-3.46701900
H	1.75100700	0.91703100	-2.85218700
H	1.15510300	-0.72939400	-3.11228500
C	-2.97303200	-0.53283900	-2.49979000
H	-2.03561300	-1.05814200	-2.31606200
C	-0.29204800	3.52332700	-0.99519800
H	0.04941300	2.76576100	-0.28603200
C	1.41390000	-1.49724500	1.89865100
O	1.98064500	-2.07298900	2.67211400
C	-0.84550500	-1.83777500	0.92189800
C	-1.57449100	-2.08564500	2.07964200
C	-1.20508500	-2.60296200	-0.18350000
C	-2.64599500	-2.95693200	2.14092300
C	-2.27429400	-3.48403200	-0.16198700
C	-3.00609600	-3.65448400	0.99955600
C	0.08283700	0.67694600	1.72128500
C	1.17681100	1.44052300	2.09744500
C	-1.15929300	1.26772000	1.92176400
C	1.08540000	2.72223900	2.61011900
C	-1.29610900	2.54507300	2.43755500

C	-0.17033900	3.27648500	2.78189000
C	2.38861600	-0.79181300	-0.65055000
C	2.85380700	-2.10649700	-0.63003600
C	3.34341500	0.20863300	-0.84783700
C	4.19179800	-2.41789900	-0.81237200
C	4.67837500	-0.08348700	-1.06380200
C	5.10606100	-1.40325400	-1.04256900
C	-3.89184500	-0.76727300	-1.29161900
H	-3.41223900	-0.44017100	-0.36668500
H	-4.82284500	-0.20482900	-1.41035300
H	-4.14971800	-1.82656400	-1.20132600
C	-3.58100500	-1.13605700	-3.76665600
H	-4.59504400	-0.76740700	-3.94777700
H	-2.97561000	-0.91209300	-4.64898800
H	-3.64528400	-2.22217300	-3.66147700
C	-0.81092700	4.71397700	-0.18126000
H	-1.08032000	5.55634700	-0.82454900
H	-1.69563800	4.44422200	0.40003600
H	-0.03925200	5.06812300	0.50839900
C	0.91223200	3.94185700	-1.84662000
H	1.31505600	3.09819300	-2.40965300
H	0.62461700	4.71534400	-2.56542400
H	1.71210400	4.34174100	-1.21673000
F	-0.55612700	-2.51384100	-1.34680200
F	-2.62113100	-4.14286100	-1.26315100
F	-4.04035300	-4.48092700	1.01945700
F	-3.31853800	-3.13397700	3.27149800
F	-1.23022700	-1.46160400	3.21712200
F	-2.28392100	0.63818200	1.59498300
F	-2.49883600	3.09165500	2.57639900
F	-0.29597700	4.50875500	3.25258600
F	2.17411400	3.41255300	2.93168600
F	2.41746100	0.92440300	1.95309100
F	2.96869000	1.48403800	-0.84166500
F	5.55390500	0.89060600	-1.26771900
F	6.38458500	-1.69039200	-1.23127500
F	4.59560000	-3.68085900	-0.77565500
F	2.00125300	-3.10427900	-0.38649000

[**TS-5**]
E(RωB97X-D) = -2976.55123266 a.u.

C	-3.12941200	-1.28790900	0.84188300
C	-3.56481100	-0.83615900	2.10613300
C	-4.79414600	-1.27738800	2.57841100
C	-5.58710500	-2.13600600	1.82642100
C	-5.14628000	-2.56809300	0.58928500
C	-3.91519700	-2.15976600	0.07389700
H	-5.14487900	-0.94966800	3.54991200
H	-6.54503500	-2.46707700	2.21106500

H	-5.76838200	-3.23887000	0.00549500
N	-1.92140500	-0.75783100	0.35313200
C	-0.83091500	-1.39871200	0.36594100
N	0.34396500	-0.74945300	-0.05904400
B	0.49465100	0.56467900	-0.84052400
C	-0.67202800	-2.80482800	0.89123000
H	-1.64459100	-3.18875000	1.19163600
H	-0.25181300	-3.46684300	0.13033800
H	-0.01323100	-2.82371400	1.76178300
C	-2.69913200	0.13700800	2.89190800
H	-1.65618900	-0.16796900	2.75936700
C	-3.47073000	-2.65775500	-1.29138900
H	-2.48159100	-2.24501600	-1.49348100
C	0.54160200	0.21875300	-2.50972000
O	0.44676800	0.09414300	-3.61659700
C	1.91965200	1.21832000	-0.42257300
C	3.07010700	1.22199100	-1.18936700
C	2.06723600	1.65575200	0.89093600
C	4.30424900	1.63546800	-0.71228000
C	3.27842800	2.07598000	1.40865000
C	4.40532000	2.06853600	0.59805600
C	-0.76853600	1.61188100	-0.95276400
C	-1.95001200	1.21811900	-1.58306400
C	-0.77564100	2.92408500	-0.48627200
C	-3.08974100	1.99082300	-1.65037000
C	-1.90269300	3.73565700	-0.53395800
C	-3.06940700	3.26485600	-1.10366000
C	1.55253100	-1.48830000	0.06517800
C	2.27060700	-1.51132500	1.25880200
C	2.09651300	-2.18508000	-1.00762700
C	3.49345100	-2.15225000	1.36261900
C	3.31995000	-2.82880600	-0.93224600
C	4.02386900	-2.80709700	0.26078600
C	-2.83223900	1.54865700	2.30374000
H	-2.59956300	1.53393800	1.23936600
H	-3.85314800	1.92170500	2.43212000
H	-2.14520600	2.24302500	2.79624200
C	-2.98113300	0.14941600	4.39358800
H	-3.96785300	0.56672900	4.61671300
H	-2.92917900	-0.85407000	4.82425800
H	-2.24367900	0.77581300	4.90216000
C	-4.40620000	-2.14935400	-2.39426400
H	-5.41238900	-2.56319400	-2.27717400
H	-4.48259300	-1.06138800	-2.36868100
H	-4.03455800	-2.44524600	-3.37988500
C	-3.35298400	-4.18593900	-1.33083800
H	-2.67565900	-4.55487300	-0.55616100
H	-4.32456700	-4.66443600	-1.17701500
H	-2.97122300	-4.51571400	-2.30166300
F	1.01902800	1.65168300	1.71315500

F	3.37532400	2.48066900	2.66787600
F	5.57268800	2.46848700	1.07913900
F	5.37841600	1.60925800	-1.49286900
F	3.03104900	0.76521700	-2.45689900
F	0.30803900	3.49637800	0.03830800
F	-1.85856800	4.96711400	-0.03823300
F	-4.14715200	4.03049100	-1.15623300
F	-4.18826300	1.54026000	-2.24654200
F	-1.99699400	0.03171700	-2.20895100
F	1.42153300	-2.23873500	-2.16138000
F	3.81046600	-3.46950800	-1.98413300
F	5.19357600	-3.41889500	0.35275100
F	4.15911400	-2.14453900	2.50890000
F	1.77829800	-0.91439000	2.33710300

TS-6

E(RωB97XD) = -2976.55532585 a.u.

Single imaginary frequency = -224.0626 cm^{-1}

N	-1.03776200	-0.48965300	-0.63687800
B	0.82587000	0.49609700	0.40066300
C	2.76231400	1.45285200	0.74975800
N	1.07739100	0.01317000	-1.01813900
C	2.33658400	-0.25497500	-1.65745300
C	3.04372000	0.81151900	-2.24469000
C	4.26542900	0.54091600	-2.85498400
C	4.76999000	-0.74793800	-2.90314500
C	4.05474300	-1.78920500	-2.33883000
C	2.83413700	-1.57168100	-1.70203900
H	4.82523800	1.34823200	-3.31169400
H	5.72125700	-0.94054300	-3.38599700
H	4.45520500	-2.79545700	-2.38737800
C	-0.10292100	-0.44268900	-1.52451000
C	-0.27116100	-0.70082200	-2.99105400
H	0.68391600	-0.73567600	-3.51159700
H	-0.81283300	-1.62864700	-3.16588000
H	-0.86635100	0.12164500	-3.39757200
C	2.47251500	2.21996200	-2.30130600
H	1.75539400	2.32706800	-1.48667400
C	2.09150600	-2.77147100	-1.12814100
H	1.27043000	-2.40746000	-0.50646600
O	3.62243800	2.09035500	1.08485400
C	0.08576100	1.90748200	0.64704200
C	-0.60176800	2.63430100	-0.32217700
C	0.11066200	2.50002600	1.90893800
C	-1.23966100	3.83547800	-0.06075400
C	-0.51409100	3.69696100	2.21082100
C	-1.20151100	4.36945800	1.21470500
C	0.88843400	-0.56117000	1.60545800
C	-0.25481300	-0.88160500	2.33403300
C	2.02801500	-1.27465100	1.94640100

C	-0.27700500	-1.88473500	3.28922900
C	2.05003700	-2.27423800	2.90361700
C	0.88119600	-2.59013700	3.57324800
C	-2.34227800	-0.86724000	-0.90621700
C	-3.39810400	0.01558500	-0.67664600
C	-2.68322700	-2.17298300	-1.26310700
C	-4.71936000	-0.36866500	-0.83099100
C	-3.99849700	-2.57347200	-1.42408700
C	-5.02393300	-1.66781000	-1.20615600
F	-0.69443900	2.20654800	-1.58547100
F	-1.88984000	4.47363300	-1.02725000
F	-1.80582600	5.51798600	1.47811300
F	-0.44902200	4.20748500	3.43515800
F	0.79810500	1.92314300	2.90508600
F	-1.39418000	-0.21722100	2.14883900
F	-1.39773000	-2.16874000	3.94348300
F	0.87283300	-3.54900900	4.48796500
F	3.17491300	-2.92891100	3.17526100
F	3.19958900	-1.00350500	1.34399400
F	-1.71505100	-3.07507400	-1.46188100
F	-4.27995900	-3.82296900	-1.77953500
F	-6.28967400	-2.04102000	-1.35821500
F	-5.69850600	0.50330400	-0.61736700
F	-3.14341900	1.26669100	-0.29776500
C	2.98549100	-3.66127100	-0.25129400
H	3.56845100	-3.08697200	0.46657700
H	2.36766100	-4.37683200	0.29790400
H	3.68419700	-4.24108800	-0.86112500
C	1.49000200	-3.63055600	-2.25011600
H	0.81733500	-3.06452500	-2.89227700
H	2.28446200	-4.04194800	-2.88030600
H	0.92661000	-4.46502400	-1.82566000
C	1.69557200	2.42081500	-3.60875500
H	2.36768100	2.32924400	-4.46742900
H	0.90225200	1.68138600	-3.71652300
H	1.23645200	3.41247200	-3.63387100
C	3.52644800	3.32001200	-2.14133200
H	4.16876200	3.15418600	-1.27396400
H	4.16882200	3.39474200	-3.02295200
H	3.03328700	4.28787900	-2.02068100

IN-2

E(RωB97X-D) = -2976.56361779 a.u.

C	-2.33106900	0.45774900	-1.62808600
C	-3.07645700	-0.52441300	-2.31099600
C	-4.27000800	-0.14976100	-2.92293400
C	-4.71243300	1.16147900	-2.88126500
C	-3.96263100	2.12050500	-2.22254900
C	-2.76964300	1.79732400	-1.57935400
H	-4.85445400	-0.89168200	-3.45413100

H	-5.64125300	1.43708000	-3.36752400
H	-4.31473500	3.14557200	-2.19966000
N	-1.11657200	0.07442900	-0.95812900
C	0.10226000	0.52031900	-1.39950100
N	1.05357200	0.51043100	-0.53804900
B	-1.12853300	-0.60901400	0.41264500
C	0.27715300	0.84743400	-2.85786500
H	-0.67214000	0.95802800	-3.37779600
H	0.86577000	1.75370200	-2.98896900
H	0.82967600	0.01817700	-3.30860200
C	-2.57397800	-1.95229900	-2.46643700
H	-1.83939600	-2.14471300	-1.68440500
C	-1.98389200	2.91247900	-0.90217200
H	-1.19333400	2.46191400	-0.29775300
C	-2.68633000	-1.17094000	0.59588300
O	-3.64853900	-1.69525100	0.81892700
C	-0.34675900	-2.04643100	0.55392700
C	-0.41766900	-2.73622200	1.76070500
C	0.42943700	-2.65749000	-0.42547900
C	0.26187800	-3.91098900	2.02171500
C	1.12987400	-3.83317700	-0.20366400
C	1.05222900	-4.46143800	1.02639300
C	-0.92160100	0.38537300	1.69247600
C	0.28360600	0.53184900	2.37301300
C	-1.94212900	1.22592700	2.10548200
C	0.47237700	1.50800500	3.33966800
C	-1.80009100	2.20585300	3.07061900
C	-0.56939400	2.35380600	3.68599200
C	2.35373700	0.86808100	-0.84893800
C	3.38224800	-0.07263700	-0.77546600
C	2.73013800	2.18996100	-1.09134800
C	4.70854600	0.27710700	-0.96568300
C	4.05110800	2.55716400	-1.28270400
C	5.04776000	1.59712000	-1.21944600
F	0.54397500	-2.14873600	-1.65592600
F	1.87179500	-4.36139900	-1.16948800
F	1.71370200	-5.58789100	1.24516500
F	0.15613600	-4.51334300	3.20039700
F	-1.19589100	-2.25587700	2.74672800
F	1.78956600	3.14054600	-1.14854500
F	3.09371600	-1.34790800	-0.51852400
F	4.36619400	3.82643700	-1.52395800
F	6.31908900	1.93846700	-1.40427300
F	5.66030500	-0.64840000	-0.90305500
F	-3.16566400	1.09496100	1.54600100
F	-2.81906800	2.99133300	3.40574700
F	1.31769600	-0.27114300	2.14065600
F	1.64685000	1.63320600	3.94798600
F	-0.39378400	3.28547200	4.61240800
C	-1.31970800	3.82181000	-1.94676700

H	-2.08044400	4.32482700	-2.55188800
H	-0.71879200	4.58782900	-1.45108500
H	-0.66695800	3.27100000	-2.62181800
C	-2.85261600	3.77716800	0.02312100
H	-3.51880700	4.42601000	-0.55283300
H	-3.46645600	3.17982300	0.69482800
H	-2.21367100	4.42705600	0.62690900
C	-1.83603200	-2.10603900	-3.80243400
H	-1.42324100	-3.11349100	-3.89969500
H	-2.52058100	-1.93053800	-4.63783700
H	-1.01247300	-1.39609200	-3.88205500
C	-3.67309800	-3.01163800	-2.33963800
H	-3.22240100	-4.00680600	-2.30814500
H	-4.27108500	-2.88016400	-1.43496200
H	-4.35570300	-2.99423600	-3.19343200

TS-7
E(RωB97X-D) = -2976.51086373 a.u.
Single imaginary frequency = -238.9741 cm^{-1}

N	0.53898000	-1.04743000	-0.48994700
C	0.79594200	-0.36777500	-1.99752500
B	0.89276900	0.76729900	-0.96298600
O	0.63673700	-0.89298400	-3.02097600
C	1.66534600	-1.74627600	0.12391300
C	2.51306300	-2.57621000	-0.63102200
C	3.73222700	-2.95586100	-0.06259600
C	4.06565200	-2.60672500	1.22942000
C	3.13644500	-1.94226100	2.01713400
C	1.91935800	-1.51892900	1.49826800
H	4.41856100	-3.55721100	-0.64759700
H	5.02465500	-2.89470400	1.64454000
H	3.36480800	-1.74883900	3.05762700
C	-0.77342500	-1.53789700	-0.21246600
N	-1.60178600	-0.68604400	0.22562900
C	-1.00557800	-2.99423500	-0.47505700
H	-0.15055100	-3.57943300	-0.13694300
H	-1.90578000	-3.34864600	0.02641900
H	-1.12024500	-3.14743000	-1.55143500
C	2.13758800	-3.22087300	-1.96029900
H	1.14790300	-2.87965400	-2.25051700
C	0.86499200	-0.95001300	2.43723500
H	0.25527100	-0.22840100	1.89186900
C	-0.26624000	1.86710400	-1.04370100
C	-0.08947400	3.19594000	-0.65091300
C	-1.50816500	1.60473400	-1.62676900
C	-1.09934000	4.14632600	-0.70739500
C	-2.54323600	2.51820400	-1.68352300
C	-2.34040300	3.80345200	-1.21015400
C	2.31091000	1.07963200	-0.32860700
C	2.44366900	1.60534700	0.95113900

C	3.49471400	0.74478100	-0.96922900
C	3.66958100	1.77754100	1.56582300
C	4.73959000	0.87638900	-0.37793400
C	4.82450200	1.39349000	0.90279300
C	-2.94339800	-0.96882300	0.45800700
C	-3.82610000	-1.46853600	-0.49970700
C	-3.48615600	-0.58160000	1.68552100
C	-5.18161100	-1.60090500	-0.23946400
C	-4.83295800	-0.72509200	1.96386900
C	-5.68792000	-1.23089600	0.99495500
F	-1.75595800	0.41996400	-2.19181400
F	-3.71569500	2.17747100	-2.20899400
F	-3.31374900	4.69858100	-1.26542400
F	-0.87181700	5.38924900	-0.29770500
F	1.08897200	3.65176600	-0.22779300
F	-2.68862200	-0.07601400	2.62207100
F	-3.37843100	-1.82878300	-1.70160400
F	-5.31387200	-0.37187200	3.14960300
F	-6.98166000	-1.36478300	1.25343300
F	-5.99367600	-2.08454700	-1.17135400
F	3.46499700	0.25652100	-2.21452200
F	5.84102300	0.51370100	-1.02493000
F	1.35873300	1.94143200	1.65079200
F	3.75112700	2.27663500	2.79619000
F	6.00397300	1.52841400	1.49026000
C	-0.05460700	-2.09213700	2.90779100
H	0.52165500	-2.82524500	3.48004400
H	-0.84398400	-1.69513900	3.54971900
H	-0.53064300	-2.62162400	2.08209600
C	1.42776600	-0.25491900	3.68102000
H	1.83208400	-0.97848300	4.39519000
H	2.20991400	0.46604300	3.45055300
H	0.62187100	0.28162400	4.18641000
C	2.04224900	-4.74475800	-1.78185300
H	1.65811900	-5.20224300	-2.69771000
H	3.02029300	-5.18656400	-1.57347200
H	1.37512000	-5.01788700	-0.96021200
C	3.10215800	-2.88264800	-3.10066700
H	2.75481800	-3.34130100	-4.03000100
H	3.18146100	-1.80876400	-3.25959400
H	4.10562400	-3.26742000	-2.89594800

IN-3

E(RωB97X-D) = -2976.54418207 a.u.

C	1.84941400	2.63084100	0.29470700
C	2.82566800	2.39734300	1.27709900
C	3.76583400	3.39824100	1.50447900
C	3.74061200	4.58097100	0.78101800
C	2.77116100	4.78532300	-0.18588900
C	1.80615200	3.81534100	-0.45139000

H	4.53093000	3.25241600	2.25829500
H	4.48398000	5.34655800	0.97282300
H	2.76178400	5.71387900	-0.74602500
N	0.84954500	1.61782000	0.06234600
C	-0.45215100	1.77805700	0.48934900
N	-1.33768200	1.16614000	-0.20687400
B	0.92765700	-0.89301300	-0.74500300
C	-0.72718900	2.66176700	1.67066700
H	-0.77089600	2.05646400	2.57736000
H	0.04196100	3.42165700	1.79541400
H	-1.69728500	3.14369800	1.54180800
C	2.85160500	1.12876000	2.11529300
H	2.25197800	0.37501200	1.59881500
C	0.74231700	4.08079500	-1.50442600
H	0.11350300	3.19521400	-1.59780900
C	1.06150700	0.67896400	-1.02930800
O	1.46467800	1.05018500	-2.09728000
C	2.24052900	-1.72871800	-0.63606100
C	3.51363600	-1.13947100	-0.62478500
C	2.23562100	-3.13121800	-0.57009100
C	4.68437200	-1.86529300	-0.50766700
C	3.39102200	-3.88462300	-0.46050000
C	4.62091200	-3.24694300	-0.42240100
C	-0.48878900	-1.55320500	-0.61167500
C	-1.43656100	-1.45360200	-1.61963700
C	-0.88593300	-2.16170500	0.56773200
C	-2.72456200	-1.93503500	-1.46887500
C	-2.16809200	-2.64596800	0.75841900
C	-3.08996700	-2.53021400	-0.27017200
C	-2.65158000	0.99510900	0.18897900
C	-3.66018800	1.20458600	-0.75647300
C	-3.03621200	0.41559100	1.39884900
C	-4.97611100	0.85811900	-0.50836800
C	-4.34759800	0.05451400	1.65973100
C	-5.32349200	0.27570000	0.70270300
C	4.26292700	0.55960700	2.30357800
H	4.20271400	-0.43751100	2.74884300
H	4.80428600	0.48809900	1.36031600
H	4.85650000	1.17822900	2.98240400
C	2.20480200	1.36650200	3.48620600
H	2.18649000	0.43963800	4.06595200
H	2.77194200	2.11157400	4.05236100
H	1.18059200	1.72794700	3.39370400
C	1.37175100	4.31703400	-2.88054800
H	0.58953700	4.44539500	-3.63355300
H	1.99529100	5.21633700	-2.88959200
H	1.98601300	3.46227200	-3.16687600
C	-0.16055200	5.24916500	-1.09063900
H	0.40288200	6.18432800	-1.01876200
H	-0.95417500	5.39160800	-1.82887500

H	-0.63021500	5.06787800	-0.11986700
F	3.33336300	-5.20776600	-0.39624800
F	1.10191600	-3.81839000	-0.62461800
F	5.72867100	-3.95385900	-0.31215400
F	5.86047400	-1.25262900	-0.47467500
F	3.65540500	0.17619400	-0.71065000
F	-0.01840500	-2.25280100	1.58337600
F	-2.53031400	-3.18537400	1.91585100
F	-4.33180000	-2.96087800	-0.09634900
F	-3.62090500	-1.80078900	-2.43994000
F	-1.11313100	-0.85976500	-2.76556600
F	-2.10929800	0.12291500	2.32049700
F	-4.66438500	-0.51783000	2.81514500
F	-6.58338200	-0.06222900	0.94295400
F	-5.90984300	1.07308800	-1.42635900
F	-3.34411700	1.72868600	-1.93473000

[TS-8]
E(RωB97X-D) = -2976.54369946 a.u.

C	1.97194200	2.61458300	0.22407200
C	2.96083900	2.43263500	1.20508700
C	3.90842700	3.44042100	1.36251900
C	3.87946900	4.57979400	0.57347900
C	2.89318500	4.73715600	-0.38518100
C	1.91800600	3.76065900	-0.57954300
H	4.68203000	3.33401200	2.11440400
H	4.63012400	5.35025900	0.70938900
H	2.87667600	5.63505900	-0.99306900
N	0.96601400	1.59495500	0.05419300
C	-0.31966300	1.76830900	0.52488000
N	-1.22439800	1.15333900	-0.14130500
B	0.85209800	-0.92149900	-0.74045800
C	-0.55457200	2.66096600	1.70611100
H	-0.56527600	2.06021200	2.61735800
H	0.21803900	3.42221600	1.79681500
H	-1.52893700	3.14133300	1.60815400
C	2.99275600	1.22378600	2.12742000
H	2.33836100	0.45944100	1.70071100
C	0.82498900	3.98556400	-1.61207600
H	0.19579800	3.09661400	-1.65786000
C	1.11266200	0.63404500	-1.01869200
O	1.56061200	0.95157000	-2.08801500
C	2.11905500	-1.82955800	-0.60412700
C	3.41811900	-1.30447100	-0.53510100
C	2.04760800	-3.23162600	-0.57707200
C	4.54935500	-2.08726900	-0.39726600
C	3.16200500	-4.04202300	-0.44755200
C	4.41841100	-3.46564300	-0.35012600
C	-0.59139200	-1.52811300	-0.66127600

C	-1.51686900	-1.36014500	-1.68073000
C	-1.03362200	-2.15567600	0.49239400
C	-2.82729900	-1.78733800	-1.56222400
C	-2.33902500	-2.58657800	0.65024100
C	-3.23890300	-2.39838600	-0.38660800
C	-2.53700700	1.02623500	0.28004400
C	-3.55622000	1.28636400	-0.64045300
C	-2.91581000	0.45428000	1.49438400
C	-4.87945200	0.99214800	-0.36525200
C	-4.23486300	0.14609000	1.78330300
C	-5.22187000	0.41431800	0.84962400
C	4.39550900	0.62120200	2.28036700
H	4.32956400	-0.34728600	2.78429600
H	4.88788100	0.47923600	1.31937200
H	5.03664700	1.25954700	2.89473600
C	2.44261600	1.58543400	3.51439500
H	2.42301200	0.70303200	4.15997100
H	3.07696000	2.33895600	3.99087800
H	1.43204500	1.99045500	3.46180600
C	1.41158400	4.18111300	-3.01290800
H	0.60682900	4.27789200	-3.74656800
H	2.02594300	5.08488400	-3.07061800
H	2.02505200	3.32217600	-3.28838100
C	-0.07149400	5.16215500	-1.20673600
H	0.49025700	6.10057400	-1.17488300
H	-0.88521200	5.28128600	-1.92703400
H	-0.51443900	5.00503000	-0.21911700
F	3.03976300	-5.36212700	-0.42159000
F	0.88719400	-3.86541000	-0.69205900
F	5.48740200	-4.22763000	-0.22187200
F	5.75171700	-1.53254200	-0.31439500
F	3.62614300	0.00455800	-0.58961900
F	-0.18940700	-2.31484500	1.51898200
F	-2.74380900	-3.13912400	1.78758500
F	-4.50242200	-2.77395200	-0.24318400
F	-3.70248900	-1.58201200	-2.53991800
F	-1.15165800	-0.74291300	-2.80126900
F	-1.97885400	0.12382500	2.39172900
F	-4.54993000	-0.41902900	2.94249200
F	-6.48861100	0.12686500	1.11671100
F	-5.82413900	1.25205200	-1.25989700
F	-3.24411500	1.80554400	-1.82220100