Electronic Supplementary Material (ESI) for Organic & Biomolecular Chemistry.

Supporting Information

Computational investigations of NHC-backbone configurations for applications in organocatalytic umpolung reactions

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CONTENTS

1. **Assessment of DFT Methods**

1.1 Comparisons of functional and basis set combinations

The free energy profiles leading to the benzoin product are calculated and discussed in the following sections. The impact upon these quantities of the functional and basis set combinations are first explored. The overall reaction profile modeled at the B3LYP/6-31G(d)/IEF-PCM-DMSO level of theory is shown in **Figure S1**. The NHC adds to the carbonyl carbon of the aldehyde to afford a zwitterionic compound (**INT1**) via transition state **TS1**, generating a new C–C single bond. The reaction energy barrier to reach **TS1** ranges from 21.1 – 25.7 kcal/mol depending on the NHC catalyst. Previous calculations indicate that the rate determining step is the first hydrogen transfer process, **TS2** (**Figure S1**). The energy barriers for this vary greatly in the present work, from 27.5 – 39.7 kcal/mol, predicting inaccessibly high barriers for carbenes **A**, **B**, and **E**, which would be inconsistent with observed reactions at typical experimental conditions. Previous literature reveals that the most favorable mechanism for the transformation from **TS2** to the Breslow intermediate (**BINT**) is through participation of protic molecules, e.g., the incorporation of solvent to shuttle protons lowers the reaction energy barrier to access **BINT** versus direct proton transfer.

1.1.1 B3LYP/6-31G(d)/IEF-PCM-DMSO

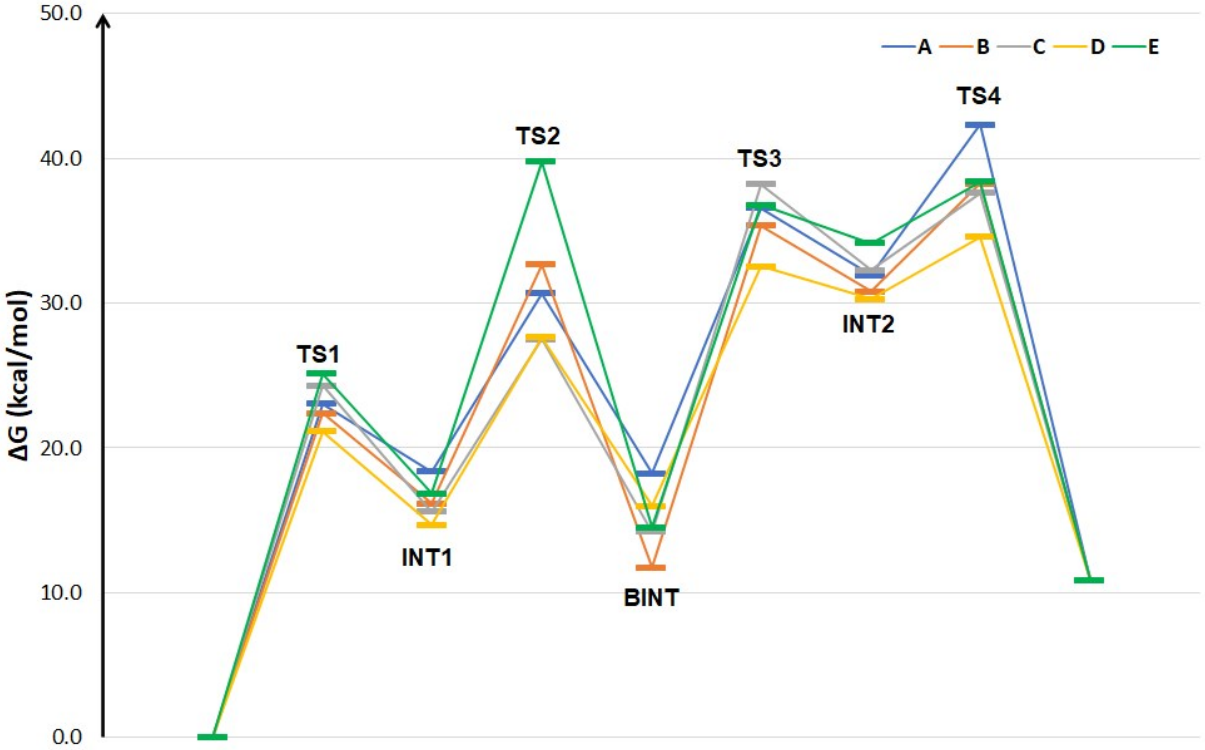

Figure S1. The Gibbs free energy (kcal/mol) profile of benzoin condensation catalyzed by N-heterocyclic carbenes calculated at the B3LYP/6-31G(d)/IEF-PCM-DMSO level of theory.

	REACT	TS1	INT1	TS2	BINT	TS3	INT2	TS4	PROD
A	0.0	23.0	18.4	30.7	18.2	36.6	31.9	42.3	10.9
B	0.0	22.4	16.2	32.7	11.8	35.3	30.8	38.3	10.9
C	0.0	24.3	15.6	27.5	14.2	38.2	32.3	37.6	10.9
D	0.0	21.1	14.7	27.6	16.0	32.5	30.3	34.6	10.9
E	0.0	25.1	16.9	39.7	14.5	36.8	34.2	38.4	10.9

Table S1. Relative free energies (kcal/mol) calculated at the B3LYP/6-31G(d)/IEF-PCM-DMSO level for benzoin condensation.

Following the hydrogen transfer process at **TS2**, the formation of the C=C double bond yields what is known as the Breslow intermediate (**BINT**), which the literature suggests should be accessed at a lower barrier relative to the preceding and the following steps in the cycle. The calculated free energies for the Breslow intermediate (**BINT**) range from 11.8 – 18.2 kcal/mole relative to separated reactants for the NHCs modeled. The reaction of **BINT** with another equivalent of benzaldehyde results in the formation of a second C–C bond via an intramolecular hydrogen transfer process in **TS3**, which is predicted at relative free energies ranging from 32.5 – 38.2 kcal/mol, **Figure S1**. The hydrogen transfer process at **TS3** results in a second zwitterionic intermediate, **INT2**, with the relative free energies to its formation ranging from 30.3 – 34.2 kcal/mol. The last transition state modeled, **TS4**, demonstrates high energy barriers (34.6 – 42.3 kcal/mol) with the subsequent release of the carbene and the newly formed benzoin product. The product formation is computed to be endergonic with a relative free energy of 10.9 kcal/mol.

In summary, based on the results from the initial B3LYP/6-31G(d)/IEFPCM-DMSO calculations, the calculated free energy profile predicts that the hydrogen-transfer process via **TS2** is the rate limiting step for this catalytic cycle for **E** (ΔG = 39.7 kcal/mol). **TS4** defines the rate limiting step for carbenes **A** (ΔG = 26.2 kcal/mol), **B** (ΔG = 38.3 kcal/mol) and **D** (ΔG = 42.3 kcal/mol), but **TS3** (ΔG = 38.2 kcal/mol) for carbene **C** (**Table S1**). Additionally, the initial survey shows the computed free energies of most stationary points in the proposed mechanism to be quite sensitive to the NHC catalyst.

1.1.2 B3LYP/6-31+G(d)/IEF-PCM-DMSO

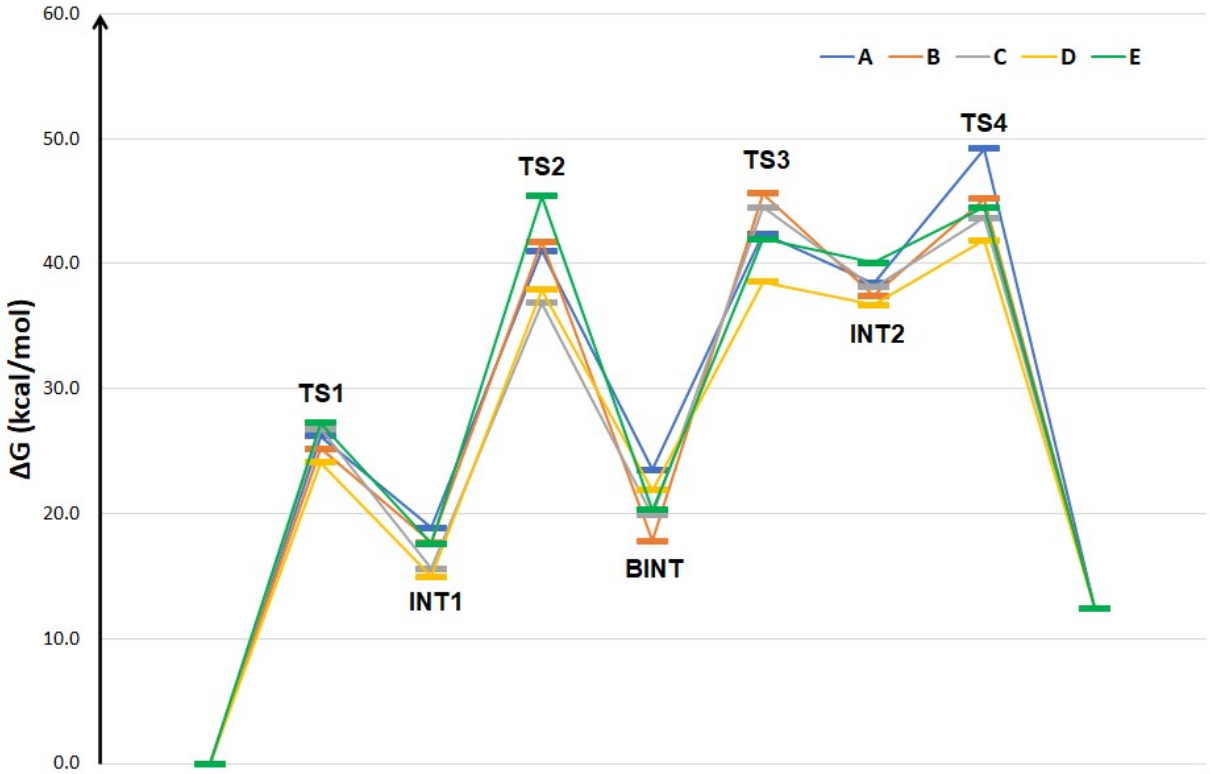

Figure S2. The Gibbs free energy (kcal/mol) profile of benzoin condensation catalyzed by N-heterocyclic carbenes calculated at the B3LYP/6-31+G(d)/IEF-PCM-DMSO level of theory.

	REACT	TS1	INT1	TS2	BINT	TS3	INT2	TS4	PROD
A	0.0	26.2	18.9	41.0	23.5	42.4	38.4	49.2	12.4
B	0.0	25.2	17.7	41.8	17.8	45.6	37.4	45.2	12.4
C	0.0	26.8	15.6	36.9	19.9	44.5	38.1	43.7	12.4
D	0.0	24.1	14.9	37.9	21.9	38.5	36.7	41.9	12.4
E	0.0	27.3	17.6	45.4	20.3	42.0	40.1	44.5	12.4

Table S2. Relative free energies (kcal/mol) calculated at the B3LYP/6-31+G(d)/IEF-PCM-DMSO level for benzoin condensation.

1.1.3 M06-2X/6-31G(d)/IEF-PCM-DMSO

Given the varying results from the initial B3LYP simulations, the NHC-catalyzed benzoin reaction was also investigated employing the M06-2X functional with the same basis sets using the same IEF-PCM-DMSO solvation model (**Figures S3-S4**). The free energies of **TS1** suggested more kinetically accessible transition states than did the previous B3LYP computations (**Tables S3-S4**).

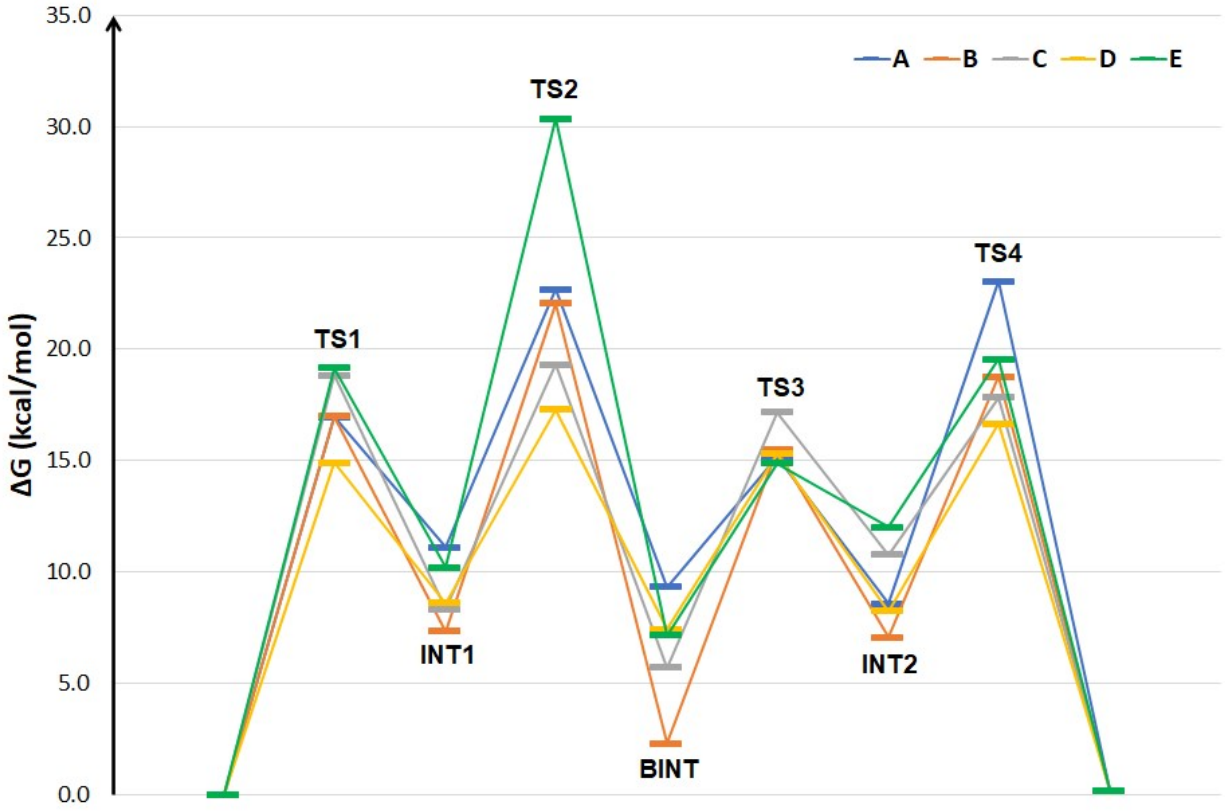

Figure S3. The Gibbs free energy (kcal/mol) profile of the benzoin condensation reaction at the M06-2X/6-31G(d)/IEF-PCM-DMSO level of theory.

	REACT	TS1	INT1	TS2	BINT	TS3	INT2	TS4	PROD
A	0.0	17.0	11.1	22.7	9.3	15.1	8.6	23.1	0.2
B	0.0	17.0	7.3	22.0	2.3	15.5	7.1	18.8	0.2
C	0.0	18.8	8.3	19.3	5.7	17.2	10.8	17.8	0.2
D	0.0	14.9	8.6	17.3	7.4	15.3	8.2	16.7	0.2
E	0.0	19.2	10.2	30.3	7.2	14.9	12.0	19.5	0.2

Table S3. Relative free energies (kcal/mol) calculated at the M06-2X/6-31G(d)/IEF-PCM-DMSO level for benzoin condensation.

1.1.4 M06-2X/6-31+G(d)/IEF-PCM-DMSO

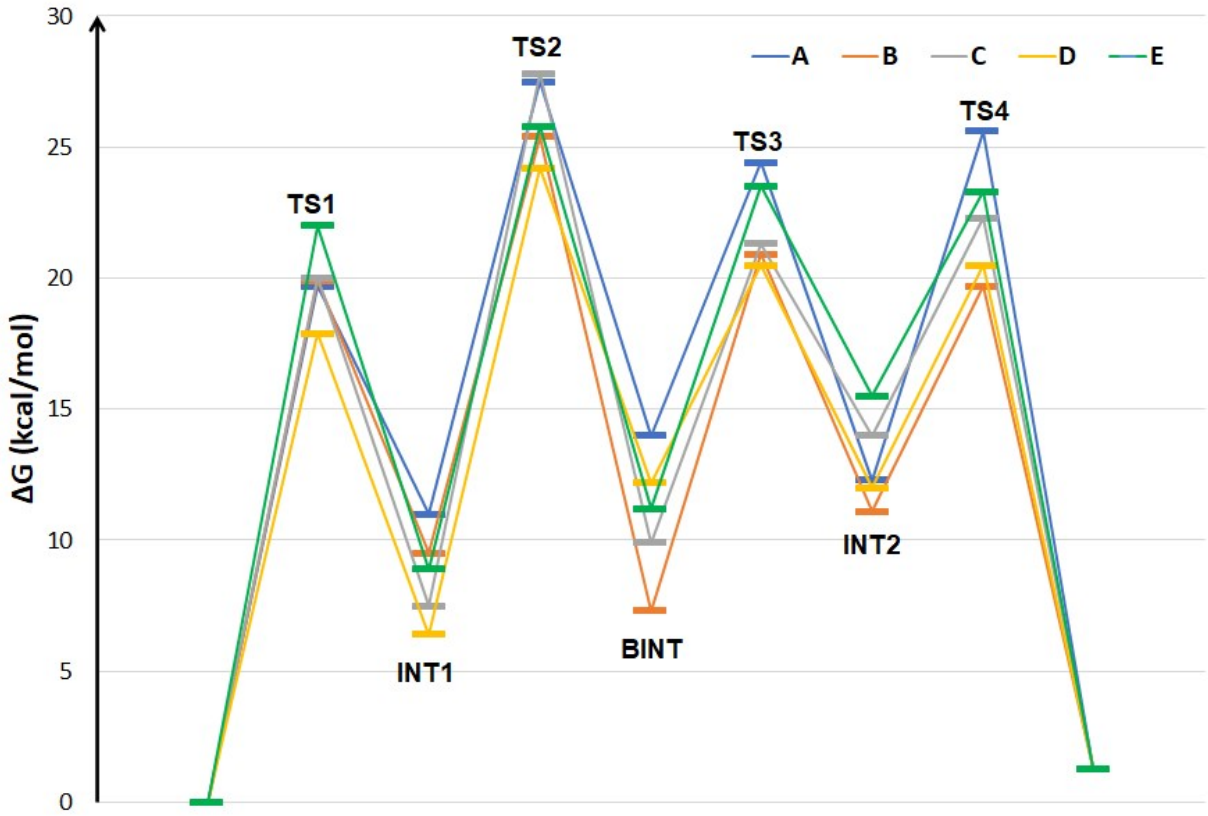

Figure S4. The Gibbs free energy (kcal/mol) profile of the benzoin condensation reaction catalyzed by N-heterocyclic carbenes calculated at the M06-2X/6-31+G(d)//IEF-PCM-DMSO level of theory.

	REACT	TS1	INT1	TS2	BINT	TS3	INT2	TS4	PROD
A	0.0	19.7	11.0	27.5	14.0	24.4	12.3	25.6	1.3
B	0.0	19.9	9.5	25.4	7.3	20.9	11.1	19.7	1.3
C	0.0	20.0	7.5	27.8	9.9	21.3	14.0	22.3	1.3
D	0.0	17.9	6.4	24.2	12.2	20.5	12.0	20.5	1.3
E	0.0	22.0	8.9	25.8	11.2	23.5	15.5	23.3	1.3

Table S4. Relative free energies (kcal/mol) calculated at the M06-2X/6-31+G(d)/IEF-PCM-DMSO level for benzoin condensation.

Considering the results presented for the previous levels of theory, M06-2X/6-31G(d) and B3LYP/6-31+G(d) were also examined (**Table S5**). It is observed that the M06-2X functional again led to more consistent results than B3LYP whereby **TS2** is the computed rate determining step for all NHC catalysts modeled. The B3LYP/6-31+G(d) calculations predicted kinetically inaccessible transition states (**Table S5**).

$G^{\ddagger}$	TS	M06-2X/ 6-31+G(d)	TS	M06-2X/ 6-31G(d)	TS	B3LYP/ 6-31G(d)	TS	B3LYP/ 6-31+G(d)
A	**2**	27.5	**2**	22.7	**4**	26.2	**4**	49.2
B	**2**	25.4	**2**	22.0	**4**	38.3	**3**	45.6
C	**2**	27.8	**2**	19.3	**3**	38.2	**3**	44.5
D	**2**	24.2	**2**	17.3	**4**	34.6	**4**	41.9
E	**2**	34.2	**2**	30.3	**2**	39.7	**2**	45.4

Table S5. Rate determining steps determined at various levels of theory tested. Geometry optimization and energy evaluations included continuum solvent effects with the IEF-PCM-DMSO model.

The relative free energy of **TS2** for carbene **E** is slightly higher than the other transition states at both the B3LYP/6-31G(d)/IEF-PCM-DMSO and the M06-2X/6-31+G(d)/IEF-PCM-DMSO levels of theory, see **Figure S1** and **Figure S4**. With the exception of this result, the transition states lie at free energies that are consistent with typical experimental conditions for NHC-catalyzed benzoin condensation. Moreover, the hydrogen-transfer process at **TS2** is observed at a lower free energy utilizing the M06-2X/6-31+G(d) combination, when compared to that of the B3LYP/6-31G(d) results and is thus more consistent with experimental reaction conditions.

The lowest activation energy for the RDS is computed for **B** (24.2 kcal/mol) followed by **B** (25.4 kcal/mol), **E** (25.8 kcal/mol), **A** (27.5 kcal/mol) and finally **C** (27.8 kcal/mol) at the M06-2X/6-31+G(d)//IEF-PCM-DMSO level of theory (**Figure S4**). It can be surmised that the results at the M06-2X/6-31+G(d)/IEF-PCM-DMSO level of theory demonstrate an overall favorable reaction profile that is consistent with experimentally-observed reactivity, also giving a slightly endergonic reaction cycle (ΔG = 1.3 kcal/mol), and the rate determining step is **TS2** as was observed in previous work (**Figure S4** and **Figure S5**).

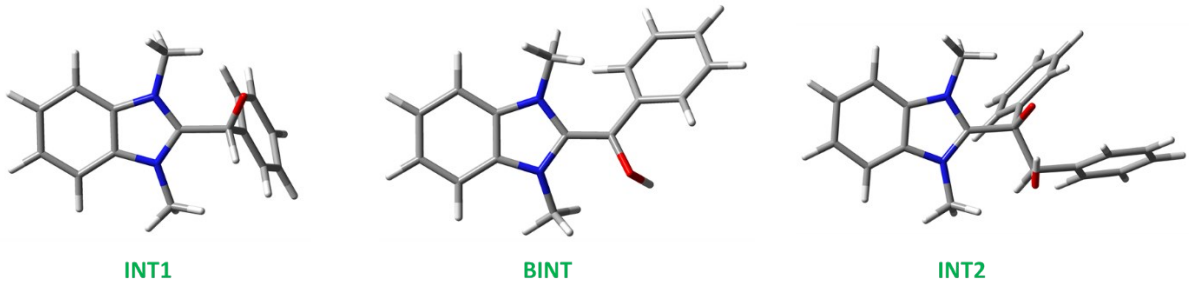

Figure S5. Calculated geometric intermediate structures of the *N,N'*-dimethylbenzimidazolylidene (**B**) involved in the NHC-catalyzed benzoin condensation.

1.1.5 M06-2X/6-311++G(d,p)/IEF-PCM-DMSO//M06-2X/6-31+G(d)/IEF-PCM-DMSO

For more accurate energetics, the larger 6-311++G(d,p) basis set was incorporated via single point calculations based on M06-2X/6-31+G(d)/IEF-PCM-DMSO-optimized geometries, **Table S5**. The energetic trends thus obtained are consistent with previous predictions. The overall catalytic process was

found to be thermoneutral when free energies were obtained at the M06-2X/6-311++G(d,p)/IEF-PCM-DMSO//M06-2X/6-31+G(d)/IEF-PCM-DMSO level of theory (**Figure S6**).

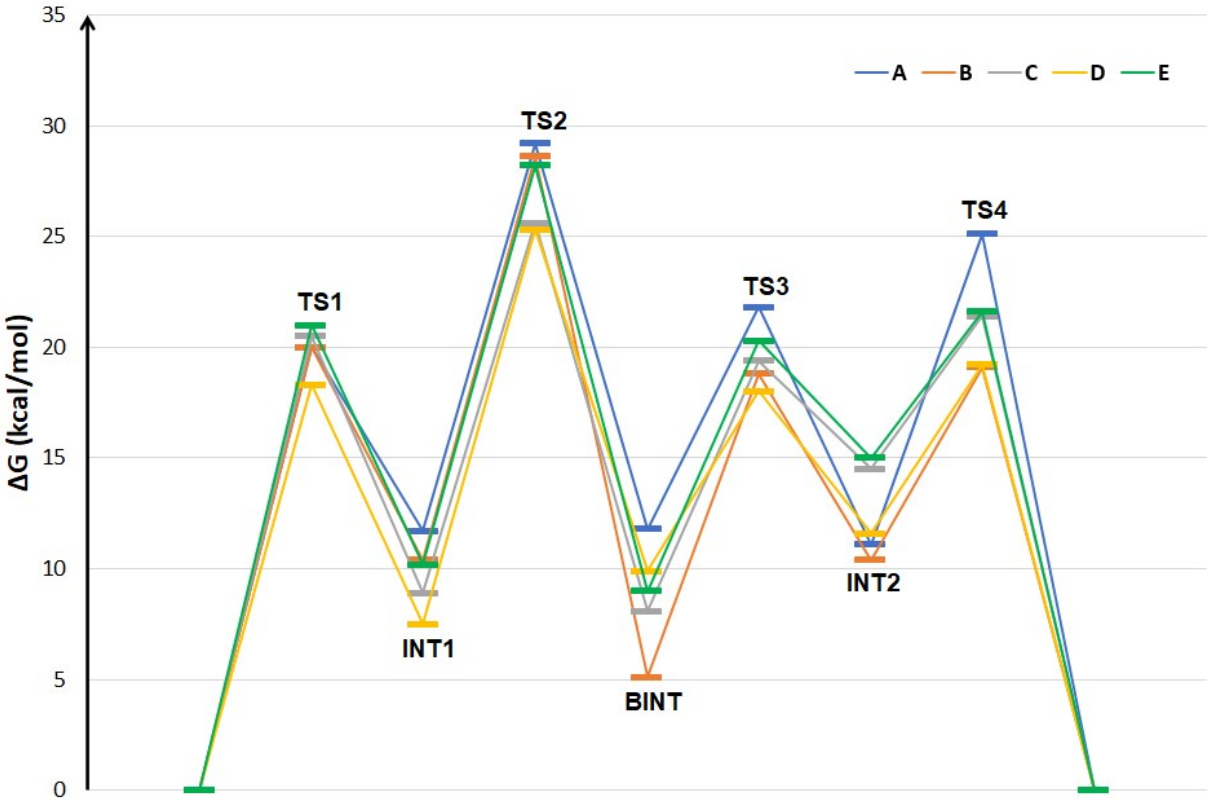

Figure S6. The Gibbs free energy (kcal/mol) profile of the benzoin condensation reaction at the M06-2X/6-311++G(d,p)/IEF-PCM-DMSO//M06-2X/6-31+G(d)/IEF-PCM-DMSO level of theory.

	REACT	TS1	INT1	TS2	BINT	TS3	INT2	TS4	PROD
A	0.0	20.0	11.7	29.2	11.8	21.8	11.1	25.1	0.0
B	0.0	20.0	10.4	28.6	5.1	18.8	10.4	19.1	0.0
C	0.0	20.5	8.9	25.6	8.1	19.4	14.5	21.4	0.0
D	0.0	18.3	7.5	25.3	9.9	18.0	11.6	19.2	0.0
E	0.0	21.0	10.2	28.2	9.0	20.3	15.0	21.6	0.0

Table S6. Relative free energies (kcal/mol) calculated at the M06-2X/6-311++G(d,p)/IEF-PCM-DMSO//M06-2X/6-31+G(d)/IEF-PCM-DMSO level of theory for benzoin condensation.

Intermediate **INT2** is most stable for carbene **B** (G_{INT2} = 10.4 kcal/mol), directly followed by **A** (G_{INT2} = 11.1 kcal/mol) and **D** (ΔG_{INT2} = 11.6 kcal/mol), **Figure S6**. Carbenes **C** and **E** resulted in higher relative free energies for this intermediate, (G_{INT2} = 14.5 kcal/mol and ΔG_{INT2} = 15.0 kcal/mol, respectively). The relative free energy for the step leading to product formation and catalyst regeneration,

TS4, is very similar for carbenes **B** - **E**, where the lowest free energy resulted from carbene **B** ($G^{\ddagger}_{TS4}$ = 19.1 kcal/mol), followed by **D** ($G^{\ddagger}_{TS4}$ = 19.2 kcal/mol), **C** ($G^{\ddagger}_{TS4}$ = 21.4 kcal/mol), **E** ($G^{\ddagger}_{TS4}$ = 21.6 kcal/mol), and the highest energy **TS4** was with carbene **A** ($G^{\ddagger}_{TS4}$ = 25.1 kcal/mol).

1.1.6 Free energy diagram of *N,N'*-dimethylbenzimidazolylidene at all levels of theory

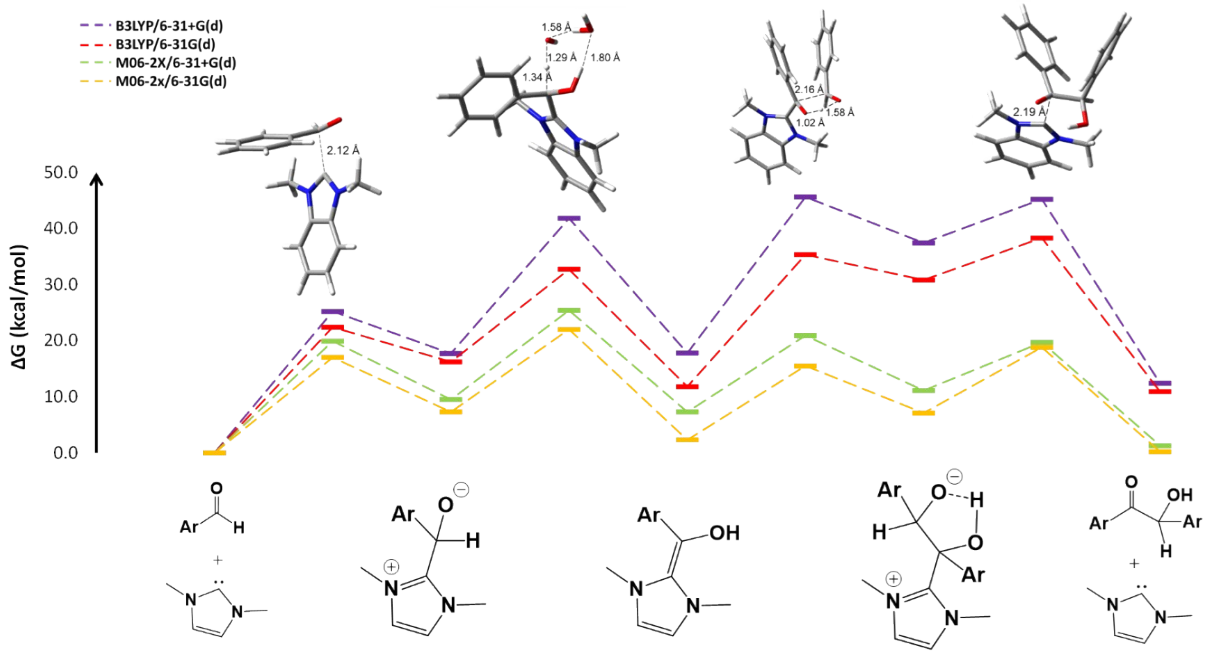

Figure S7. The Gibbs free energy (in kcal/mol) profile of the benzoin condensation catalyzed by *N,N'*-dimethylbenzimidazolylidene at different levels of theory. All simulations employed the IEF-PCM-DMSO continuum solvation model.

1.2 Comparison of DCM vs. DMSO Solvation

1.2.1 M06-2X/6-31+G(d)/IEF-PCM-DCM

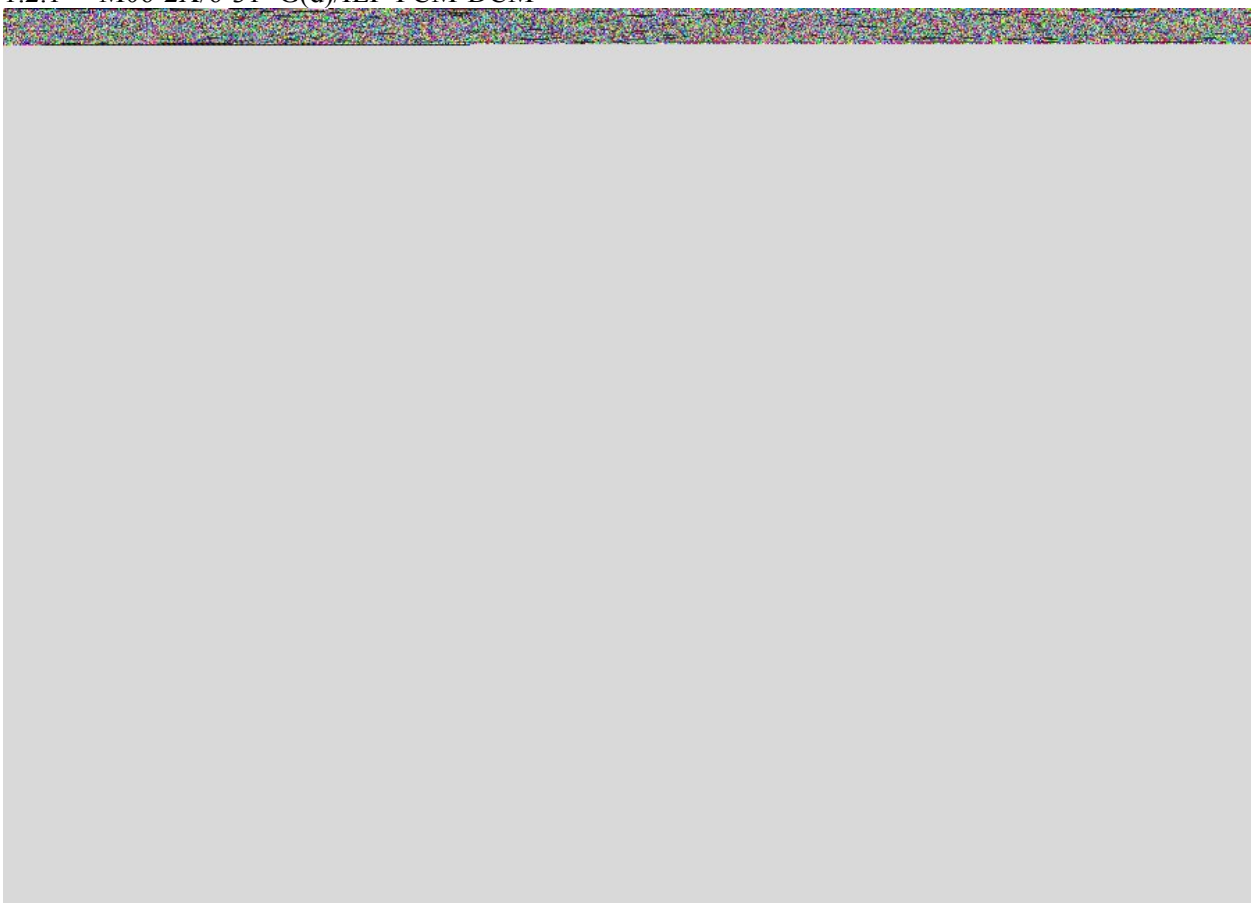

Figure S8. The Gibbs free energy (kcal/mol) profile of benzoin condensation catalyzed by N-heterocyclic carbenes calculated at the M06-2X/6-31+G(d)/IEF-PCM-DCM level of theory.

1.2.2 M06-2X/6-31+G(d)/IEF-PCM-DMSO

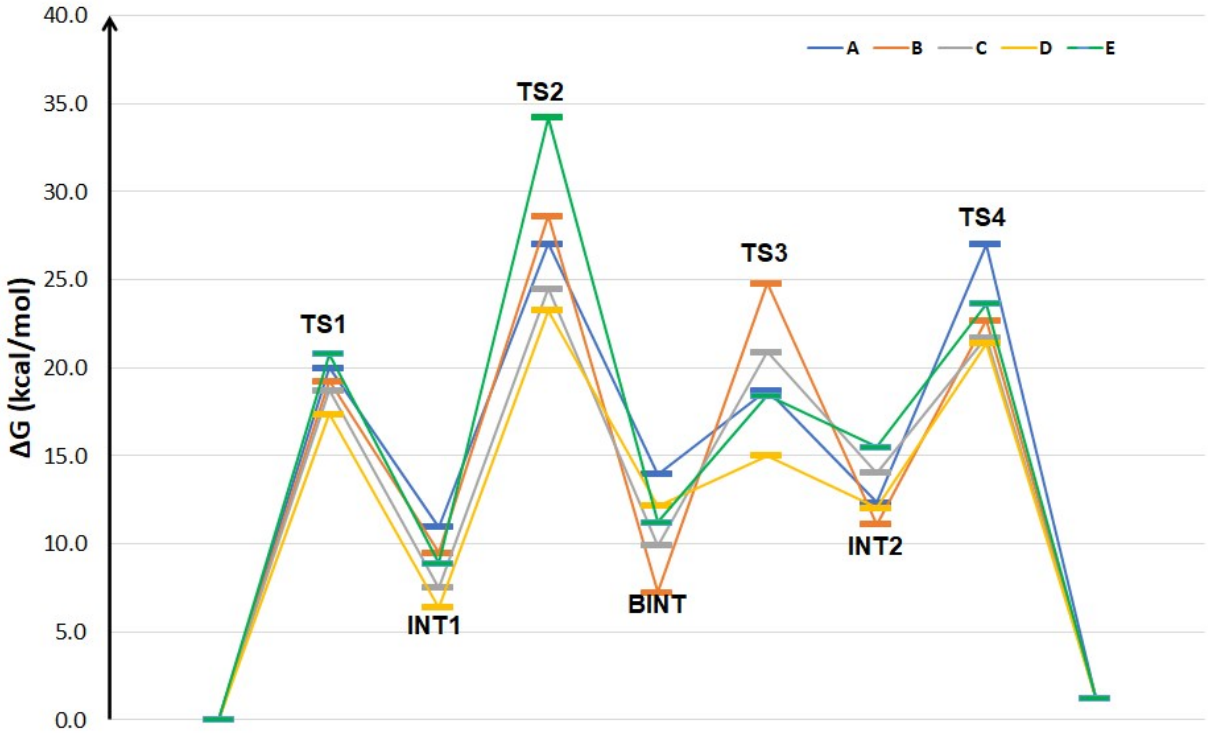

Figure S9. The Gibbs free energy (kcal/mol) profile of the benzoin condensation reaction catalyzed by N-heterocyclic carbenes calculated at the M06-2X/6-31+G(d)//IEF-PCM-DMSO level of theory.

1.3 DFT Calculations

1.3.1 HOMO-LUMO Energy Diagram

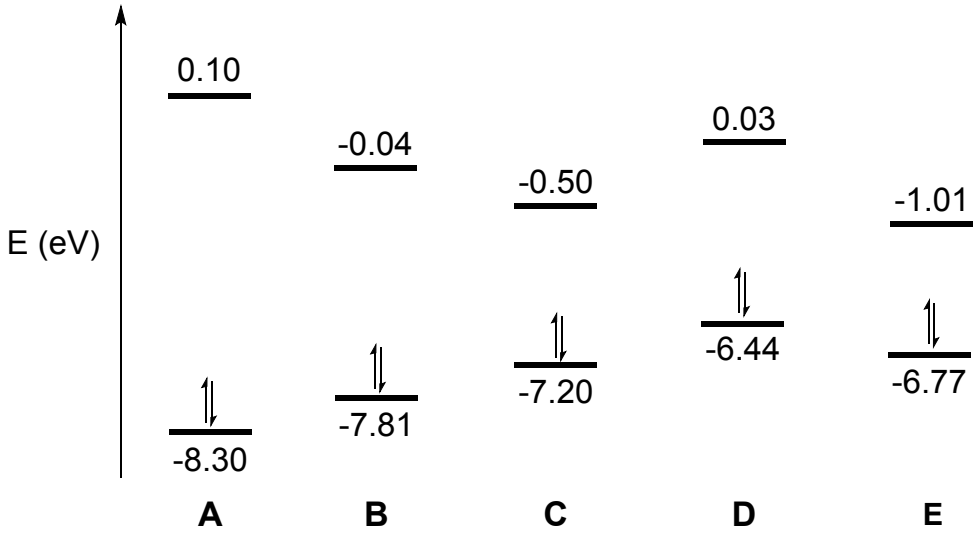

Figure S10. M06-2X/6-311++G(d,p) calculated HOMO-LUMO energies (eV).

1.4 Reactions Pathways from INT1 to BINT

1.4.1 Intermolecular proton transfer

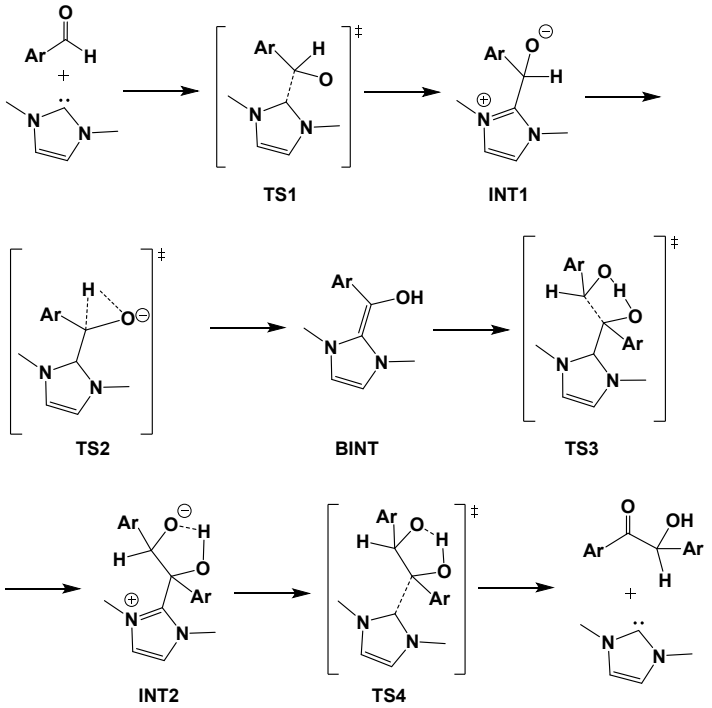

Figure S11. Intramolecular proton transfer pathway for the benzoin condensation.

1.4.2 Water-assisted proton transfer

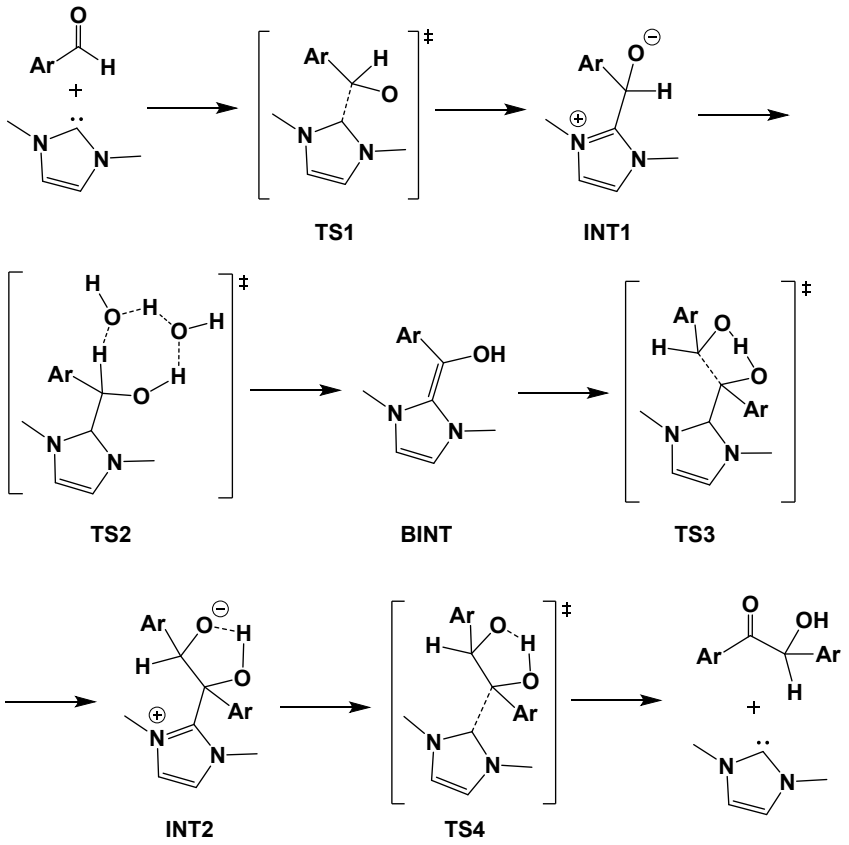

Figure S12. Water-assisted proton transfer pathway for the benzoin condensation.

1.5 List of absolute energies of optimized structures

M06-2X/6-311++G(d,p)/IEF-PCM-DMSO//M06-2X/6-31+G(d)/IEF-PCM-DMSO

Compounds	E (a.u.)	ZPE (a.u.)	G (a.u.)	ΔG (kcal/mol)
Benzaldehyde	-345.527447	-345.417091	-345.447477	
Benzoin	-691.080390	-690.855102	-690.895032	
H2O	-76.4293049	-76.4080260	-76.4256730	
	E (a.u.)	ZPE (a.u.)	G (a.u.)	ΔG (kcal/mol)
A + Benzaldehyde	-705.646637	-705.392016	-705.454434	0.0
TS1	-705.636746	-705.380313	-705.422587	20.0
INT1	-705.653071	-705.435807	-705.435807	11.7
TS2 (INT1 + 2H2O)	-858.517007	-858.212732	-858.259320	29.2
BINT	-705.652226	-705.394592	-705.435612	11.8
TS3 (BINT + Benzaldehyde)	-1051.196143	-1050.820249	-1050.867221	21.8
INT2	-1051.208323	-1050.835442	-1050.884167	11.1

TS4	-1051.183551	-1050.812416	-1050.861936	25.1
Benzoin + A	-1051.199581	-1050.830027	-1050.901989	0.0

	E (a.u.)	ZPE (a.u.)	G (a.u.)	ΔG (kcal/mol)
B + Benzaldehyde	-803.9219071	-803.6364131	-803.7005091	0.0
TS1	-803.9131636	-803.6256310	-803.6686590	20.0
INT1	-803.9296647	-803.6406734	-803.6839755	10.4
TS2 (INT1 + 2H2O)	-956.7958485	-956.4606658	-956.5084564	28.6
BINT	-803.9390465	-803.6500916	-803.6923891	5.1
TS3 (BINT + Benzaldehyde)	-1149.470870	-1149.069117	-1149.118081	18.8
INT2	-1149.485478	-1149.081328	-1149.131436	10.4
TS4	-1149.467555	-1149.065893	-1149.117591	19.1
Benzoin + B	-1149.474851	-1149.074424	-1149.148064	0.0

	E (a.u.)	ZPE (a.u.)	G (a.u.)	ΔG (kcal/mol)
C + Benzaldehyde	-6259.484388	-6259.103509	-6259.183264	0.0
TS1	-6259.475190	-6259.092457	-6259.150550	20.5
INT1	-6259.495313	-6259.111098	-6259.169094	8.9
TS2 (INT1 + 2H2O)	-6412.357063	-6411.926410	-6411.989787	25.6
BINT	-6259.496548	-6259.113031	-6259.170411	8.1
TS3 (BINT + Benzaldehyde)	-6605.032960	-6604.536273	-6604.599858	19.4
INT2	-6605.040084	-6604.541365	-6604.607609	14.5
TS4	-6605.027933	-6604.531093	-6604.596712	21.4
Benzoin + C	-6605.037331	-6604.541522	-6604.630815	0.0

	E (a.u.)	ZPE (a.u.)	G (a.u.)	ΔG (kcal/mol)
D + Benzaldehyde	-650.2930102	-650.054755	-650.115466	0.0
TS1	-650.2848854	-650.045458	-650.086357	18.3
INT1	-650.3060905	-650.063967	-650.103635	7.4
TS2 (INT1 + 2H2O)	-803.1697564	-802.881090	-802.925466	25.3
BINT	-650.3018841	-650.060586	-650.099668	9.9
TS3 (BINT + Benzaldehyde)	-995.8422288	-995.488189	-995.534309	18.0
INT2	-995.8541458	-995.497033	-995.544468	11.6
TS4	-995.8372551	-995.483283	-995.532281	19.2
Benzoin + D	-995.8459533	-995.492766	-995.563021	0.0

	E (a.u.)	ZPE (a.u.)	G (a.u.)	ΔG (kcal/mol)
E + Benzaldehyde	-2857.45965	-2857.030742	-2857.117325	0.0
TS1	-2857.450413	-2857.019506	-2857.083879	21.0
INT1	-2857.468163	-2857.035955	-2857.101065	10.2
TS2 (INT1 + 2H2O)	-3010.332188	-3009.854813	-3009.925258	28.2
BINT	-2857.469748	-2857.038365	-2857.102956	9.0
TS3 (BINT + Benzaldehyde)	-3203.006411	-3202.462059	-3202.532406	20.3
INT2	-3203.015176	-3202.468291	-3202.540904	15.0
TS4	-3203.002597	-3202.457944	-3202.530410	21.6
Benzoin + E	-3203.012593	-3202.468753	-3202.56488	0.0

2. **Optimized structures of the compounds**

All of the structures, unless specified, are optimized using the M06-2X/6-311++G(d,p)/IEF-PCM-DMSO//M06-2X/6-31+G(d)/IEF-PCM-DMSO level of theory.

2.1 Coordinates of optimized structures

Benzaldehyde neutral singlet

C	-1.724867000000	1.067609000000	-0.000025000000
C	-0.348252000000	1.287798000000	0.000007000000
C	0.532557000000	0.202068000000	0.000018000000
C	0.038143000000	-1.108777000000	0.000001000000
C	-1.335058000000	-1.326345000000	-0.000027000000
C	-2.215359000000	-0.238422000000	-0.000042000000
H	-2.411541000000	1.908852000000	-0.000037000000
H	0.048531000000	2.300809000000	0.000022000000
H	0.734370000000	-1.942965000000	0.000014000000
H	-1.725515000000	-2.339757000000	-0.000039000000
H	-3.287673000000	-0.412976000000	-0.000066000000
O	2.844847000000	-0.395199000000	0.000024000000
C	1.988104000000	0.467822000000	0.000043000000
H	2.271446000000	1.537109000000	0.000064000000

Benzoin neutral singlet

C	0.548608000000	1.487150000000	-0.071249000000
O	0.667887000000	2.496971000000	0.604613000000
C	1.571581000000	0.407654000000	-0.050804000000
C	1.632251000000	-0.577627000000	-1.044554000000
C	2.500189000000	0.395961000000	0.998420000000
C	2.616350000000	-1.562543000000	-0.986808000000
H	0.931047000000	-0.575375000000	-1.873450000000
C	3.474022000000	-0.595168000000	1.058926000000
C	3.533251000000	-1.574829000000	0.064765000000
H	2.666723000000	-2.319631000000	-1.763606000000
H	4.186184000000	-0.606246000000	1.878695000000
H	4.295309000000	-2.347776000000	0.109803000000
H	2.443719000000	1.162531000000	1.765479000000
C	-3.133503000000	-1.848002000000	0.770599000000
C	-2.682122000000	-1.940196000000	-0.545548000000
C	-1.900800000000	-0.918826000000	-1.089561000000
C	-1.566318000000	0.197560000000	-0.322105000000
C	-2.023268000000	0.286909000000	0.997167000000
C	-2.804116000000	-0.730470000000	1.541582000000
H	-3.741679000000	-2.641733000000	1.195108000000
H	-2.940367000000	-2.803912000000	-1.151785000000

H	-1.550907000000	-0.988410000000	-2.117238000000
H	-1.773551000000	1.157177000000	1.601542000000
H	-3.154167000000	-0.653215000000	2.567093000000
C	-0.727322000000	1.324780000000	-0.907630000000
O	-1.431584000000	2.544073000000	-0.920341000000
H	-0.453148000000	1.070323000000	-1.937684000000
H	-1.032409000000	3.103797000000	-0.227341000000

2,4,5-trimethyl-1,2,4-triazolylidene (**A**)

Carbene neutral singlet

C	0.617842000000	0.680459000000	-0.000021000000
C	-0.608736000000	-1.208434000000	-0.000034000000
N	-1.340805000000	-0.084332000000	-0.000005000000
N	0.658647000000	-0.690621000000	0.000012000000
C	1.889892000000	-1.465794000000	0.000072000000
H	2.478523000000	-1.237370000000	0.892111000000
H	1.626605000000	-2.523007000000	0.000085000000
H	2.478581000000	-1.237408000000	-0.891939000000
N	-0.623524000000	1.082408000000	-0.000060000000
C	1.823336000000	1.550351000000	-0.000001000000
H	2.437933000000	1.358265000000	0.885436000000
H	2.438085000000	1.358093000000	-0.885294000000
H	1.518817000000	2.598511000000	-0.000128000000
C	-2.788500000000	0.014406000000	0.000001000000
H	-3.121187000000	0.549587000000	-0.892606000000
H	-3.199414000000	-0.994581000000	0.000126000000
H	-3.121164000000	0.549798000000	0.892490000000

TS1 neutral singlet, imaginary frequency = 177.6*i* cm^{-1}

C	-0.831783000000	0.077151000000	1.846824000000
O	-0.745436000000	-0.907470000000	2.603770000000
C	-1.685232000000	0.020994000000	0.599491000000
C	-2.068274000000	1.201809000000	-0.042634000000
C	-2.119003000000	-1.208473000000	0.098856000000
C	-2.867220000000	1.155173000000	-1.184051000000
H	-1.734423000000	2.159495000000	0.354294000000
C	-2.914294000000	-1.257820000000	-1.046423000000
C	-3.288558000000	-0.076818000000	-1.690599000000
H	-3.164270000000	2.076546000000	-1.677915000000
H	-3.248325000000	-2.216762000000	-1.433857000000
H	-3.910660000000	-0.114461000000	-2.580627000000
H	-1.832115000000	-2.120029000000	0.617051000000
H	-0.735709000000	1.099990000000	2.251384000000

C	2.546247000000	-0.263062000000	-0.729931000000
C	0.965234000000	0.318658000000	0.732387000000
N	1.556452000000	1.369945000000	0.162933000000
N	1.607087000000	-0.730309000000	0.156041000000
C	1.324057000000	-2.136580000000	0.416703000000
H	0.593309000000	-2.185873000000	1.224993000000
H	0.922706000000	-2.608726000000	-0.483860000000
H	2.242708000000	-2.646442000000	0.717155000000
N	2.532415000000	1.042623000000	-0.739607000000
C	3.430751000000	-1.140305000000	-1.539372000000
H	4.054170000000	-1.765123000000	-0.891763000000
H	2.835558000000	-1.801225000000	-2.177635000000
H	4.075878000000	-0.524822000000	-2.169095000000
C	1.252016000000	2.772699000000	0.380362000000
H	0.827540000000	3.203476000000	-0.529808000000
H	0.533610000000	2.843566000000	1.197033000000
H	2.168184000000	3.303782000000	0.647243000000

INT1 neutral singlet

C	-0.345102000000	0.518595000000	1.388738000000
O	-0.281374000000	-0.272182000000	2.464258000000
C	-1.545376000000	0.278451000000	0.438616000000
C	-1.767570000000	1.098208000000	-0.674114000000
C	-2.433256000000	-0.761684000000	0.705040000000
C	-2.858737000000	0.875245000000	-1.512803000000
H	-1.081958000000	1.920176000000	-0.883166000000
C	-3.529296000000	-0.989047000000	-0.132146000000
C	-3.743685000000	-0.173132000000	-1.243261000000
H	-3.022606000000	1.518273000000	-2.373618000000
H	-4.216888000000	-1.803014000000	0.083570000000
H	-4.595504000000	-0.348274000000	-1.894743000000
H	-2.247400000000	-1.379221000000	1.579863000000
H	-0.371516000000	1.609177000000	1.611678000000
C	2.531829000000	-0.597352000000	-0.629403000000
C	0.909824000000	0.347068000000	0.508998000000
N	1.763135000000	1.253158000000	0.047651000000
N	1.391059000000	-0.840723000000	0.088543000000
C	0.778111000000	-2.148676000000	0.312752000000
H	1.571767000000	-2.882867000000	0.458652000000
H	0.164955000000	-2.065157000000	1.210722000000
H	0.173482000000	-2.421183000000	-0.555770000000
N	2.776707000000	0.686012000000	-0.663502000000
C	3.353777000000	-1.658951000000	-1.262047000000
H	3.764913000000	-2.330382000000	-0.501785000000
H	2.746536000000	-2.252750000000	-1.952024000000
H	4.174749000000	-1.195939000000	-1.811670000000

C	1.731146000000	2.703819000000	0.168366000000
H	1.486013000000	3.137591000000	-0.802971000000
H	0.981115000000	2.986963000000	0.904019000000
H	2.717037000000	3.039660000000	0.491919000000

TS2 neutral singlet, imaginary frequency = 1302.8*i* cm^{-1}

N	-3.048350000000	-0.412674000000	-0.934118000000
C	-2.831847000000	-0.982392000000	0.219061000000
C	-0.966179000000	0.074382000000	-0.285501000000
N	-1.562131000000	-0.702263000000	0.655326000000
N	-1.883451000000	0.224272000000	-1.242766000000
C	0.364437000000	0.681022000000	-0.166694000000
O	0.518050000000	1.759239000000	-1.079989000000
H	0.427308000000	2.597071000000	-0.575832000000
H	0.442746000000	1.210171000000	1.076751000000
O	0.267646000000	3.928713000000	0.643433000000
O	0.547364000000	1.852125000000	2.175323000000
H	0.413478000000	3.242108000000	1.372940000000
H	1.030064000000	4.525761000000	0.665991000000
H	1.454326000000	1.721949000000	2.494101000000
C	1.514520000000	-0.275903000000	-0.238566000000
C	2.810664000000	0.260341000000	-0.145949000000
C	1.383416000000	-1.666393000000	-0.360383000000
C	3.932244000000	-0.563135000000	-0.169868000000
C	2.508691000000	-2.494238000000	-0.374249000000
C	3.787774000000	-1.949353000000	-0.278314000000
H	2.928641000000	1.338260000000	-0.061512000000
H	0.399413000000	-2.118502000000	-0.468677000000
H	4.923993000000	-0.123851000000	-0.098636000000
H	2.379520000000	-3.568892000000	-0.474478000000
H	4.662414000000	-2.593357000000	-0.293988000000
C	-1.777220000000	0.921724000000	-2.519434000000
H	-0.796948000000	0.738823000000	-2.953617000000
H	-2.558819000000	0.514338000000	-3.160449000000
H	-1.925083000000	1.993213000000	-2.375977000000
C	-0.977694000000	-1.145893000000	1.916604000000
H	-0.222505000000	-0.420566000000	2.224583000000
H	-1.768330000000	-1.181362000000	2.667962000000
H	-0.534242000000	-2.137278000000	1.797996000000
C	-3.801455000000	-1.816830000000	0.973064000000
H	-4.032796000000	-1.364498000000	1.942474000000
H	-4.722027000000	-1.902905000000	0.393220000000
H	-3.392206000000	-2.816424000000	1.149289000000

BINT neutral singlet

C	0.324219000000	0.997184000000	0.252021000000
O	0.376406000000	2.377682000000	0.499139000000
C	1.592722000000	0.326140000000	0.041033000000
C	1.723701000000	-0.819708000000	-0.777220000000
C	2.778026000000	0.857718000000	0.597873000000
C	2.958573000000	-1.430153000000	-0.974425000000
H	0.852037000000	-1.211503000000	-1.295418000000
C	4.012108000000	0.249871000000	0.385340000000
C	4.116253000000	-0.907270000000	-0.391410000000
H	3.020024000000	-2.309485000000	-1.611099000000
H	4.902334000000	0.683250000000	0.834998000000
H	5.080050000000	-1.380820000000	-0.553842000000
H	2.719120000000	1.756500000000	1.204800000000
H	0.202206000000	2.537539000000	1.441151000000
C	-2.699767000000	-0.912634000000	0.007760000000
C	-0.935331000000	0.447513000000	0.091194000000
N	-2.094566000000	1.120945000000	-0.192368000000
N	-1.340874000000	-0.870912000000	0.245712000000
C	-0.592775000000	-1.915771000000	0.923084000000
H	-0.039979000000	-2.543910000000	0.220183000000
H	0.111806000000	-1.447258000000	1.615350000000
H	-1.289657000000	-2.535086000000	1.490021000000
N	-3.170765000000	0.261497000000	-0.269747000000
C	-3.502312000000	-2.161310000000	0.090912000000
H	-3.048419000000	-2.952507000000	-0.513652000000
H	-3.568477000000	-2.518085000000	1.124137000000
H	-4.511418000000	-1.962200000000	-0.274791000000
C	-2.194116000000	2.434858000000	-0.795176000000
H	-2.000666000000	3.222874000000	-0.065742000000
H	-1.476094000000	2.526885000000	-1.617247000000
H	-3.208490000000	2.533012000000	-1.183061000000

TS3 neutral singlet, imaginary frequency = 231.6*i* cm^{-1}

C	3.566641000000	0.568897000000	0.846660000000
N	3.770814000000	-0.690493000000	0.588301000000
C	1.810191000000	-0.092311000000	-0.319986000000
N	2.687014000000	-1.090952000000	-0.126449000000
N	2.382555000000	0.987725000000	0.288491000000
C	0.532261000000	-0.221381000000	-1.017276000000
O	0.696744000000	-0.773328000000	-2.270444000000
H	0.184371000000	-1.649515000000	-2.217532000000
C	-0.397350000000	-1.976562000000	-0.161687000000
O	-0.511498000000	-2.660296000000	-1.237587000000
H	0.426709000000	-2.211599000000	0.535560000000
C	-1.606977000000	-1.479462000000	0.545823000000
C	-2.810029000000	-1.279662000000	-0.142445000000

C	-1.546212000000	-1.195747000000	1.913112000000
C	-3.925404000000	-0.779046000000	0.524753000000
C	-2.666344000000	-0.708808000000	2.587563000000
C	-3.856638000000	-0.491158000000	1.892005000000
H	-2.854431000000	-1.511804000000	-1.203366000000
H	-0.610228000000	-1.350836000000	2.448157000000
H	-4.852741000000	-0.613676000000	-0.017776000000
H	-2.609712000000	-0.495340000000	3.651602000000
H	-4.729285000000	-0.104747000000	2.411491000000
C	-0.488959000000	0.841122000000	-0.913810000000
C	-1.269109000000	1.165818000000	-2.033803000000
C	-0.820602000000	1.445549000000	0.314410000000
C	-2.329298000000	2.069821000000	-1.935219000000
C	-1.873093000000	2.347486000000	0.411322000000
C	-2.639841000000	2.667347000000	-0.714918000000
H	-1.040670000000	0.697457000000	-2.985839000000
H	-0.263873000000	1.186676000000	1.211964000000
H	-2.915830000000	2.303457000000	-2.820262000000
H	-2.108883000000	2.792171000000	1.375217000000
H	-3.467651000000	3.366391000000	-0.635891000000
C	2.702831000000	-2.449616000000	-0.655123000000
H	1.748623000000	-2.684984000000	-1.119260000000
H	3.502900000000	-2.520450000000	-1.396324000000
H	2.902315000000	-3.133435000000	0.171592000000
C	2.022283000000	2.401709000000	0.171631000000
H	2.947421000000	2.974256000000	0.096797000000
H	1.440607000000	2.549631000000	-0.735748000000
H	1.452812000000	2.731506000000	1.041916000000
C	4.483282000000	1.448893000000	1.615206000000
H	3.943391000000	1.967361000000	2.412820000000
H	5.272210000000	0.835379000000	2.053627000000
H	4.941502000000	2.199786000000	0.963790000000

INT2 neutral singlet

C	-0.239581000000	-0.165183000000	0.633925000000
O	-0.172604000000	-0.300883000000	1.977867000000
C	0.370311000000	1.136499000000	0.056627000000
C	0.149239000000	1.534870000000	-1.270609000000
C	1.192104000000	1.926117000000	0.868336000000
C	0.739960000000	2.697601000000	-1.776639000000
H	-0.486456000000	0.936851000000	-1.921606000000
C	1.789513000000	3.087729000000	0.365923000000
C	1.565390000000	3.478738000000	-0.959051000000
H	0.555226000000	2.992596000000	-2.807246000000
H	2.426469000000	3.689822000000	1.010515000000
H	2.025180000000	4.383377000000	-1.350013000000

H	1.349200000000	1.618420000000	1.897898000000
C	4.820011000000	-1.063444000000	-0.205365000000
C	4.047422000000	-0.947400000000	-1.365642000000
C	2.654724000000	-1.066467000000	-1.294817000000
C	2.008632000000	-1.297496000000	-0.070517000000
C	2.795838000000	-1.425027000000	1.085605000000
C	4.187576000000	-1.306089000000	1.020313000000
H	5.902733000000	-0.974669000000	-0.255829000000
H	4.526739000000	-0.771300000000	-2.326115000000
H	2.062765000000	-0.982320000000	-2.204097000000
H	2.315156000000	-1.617715000000	2.039520000000
H	4.779817000000	-1.404731000000	1.927546000000
C	0.494005000000	-1.430450000000	-0.021616000000
O	0.095666000000	-2.529792000000	0.790702000000
H	0.149446000000	-1.594148000000	-1.044599000000
H	-0.079498000000	-2.052418000000	1.652606000000
C	-3.876744000000	-0.456526000000	-0.355866000000
C	-1.772240000000	-0.137771000000	0.263857000000
N	-2.588389000000	0.785996000000	0.786191000000
N	-2.590929000000	-0.951410000000	-0.465638000000
C	-2.255244000000	-2.146688000000	-1.253317000000
H	-1.766232000000	-1.856988000000	-2.186244000000
H	-1.615660000000	-2.800558000000	-0.662111000000
H	-3.183521000000	-2.667910000000	-1.482929000000
N	-3.888256000000	0.606484000000	0.408803000000
C	-5.082573000000	-1.036906000000	-1.008035000000
H	-4.965645000000	-1.071915000000	-2.096855000000
H	-5.275934000000	-2.055825000000	-0.653582000000
H	-5.946192000000	-0.412821000000	-0.765718000000
C	-2.268397000000	1.902622000000	1.672354000000
H	-1.409641000000	1.616927000000	2.277949000000
H	-2.052569000000	2.797490000000	1.082145000000
H	-3.142525000000	2.077368000000	2.301914000000

TS4 neutral singlet, imaginary frequency = 174.0*i* cm^{-1}

C	0.157241000000	-0.280807000000	0.484676000000
O	0.040316000000	-0.844660000000	1.594156000000
C	0.217682000000	1.244460000000	0.477764000000
C	0.939793000000	1.994165000000	-0.454573000000
C	-0.487285000000	1.918704000000	1.481796000000
C	0.951459000000	3.389926000000	-0.387661000000
H	1.491370000000	1.509277000000	-1.253372000000
C	-0.490066000000	3.309440000000	1.542949000000
C	0.232945000000	4.052313000000	0.605339000000
H	1.520527000000	3.956541000000	-1.119902000000
H	-1.052428000000	3.816581000000	2.322529000000

H	0.236391000000	5.137914000000	0.651897000000
H	-1.041101000000	1.333833000000	2.211659000000
C	5.226498000000	-0.918484000000	0.074608000000
C	4.704862000000	-0.461593000000	-1.135109000000
C	3.325343000000	-0.476511000000	-1.348928000000
C	2.454237000000	-0.942631000000	-0.360026000000
C	2.986769000000	-1.411041000000	0.848131000000
C	4.363568000000	-1.396177000000	1.064240000000
H	6.299492000000	-0.907332000000	0.245651000000
H	5.369461000000	-0.094965000000	-1.912745000000
H	2.921057000000	-0.121222000000	-2.295149000000
H	2.310175000000	-1.781649000000	1.612558000000
H	4.765683000000	-1.758491000000	2.006631000000
C	0.958286000000	-0.995697000000	-0.624583000000
O	0.506668000000	-2.343097000000	-0.652152000000
H	0.749917000000	-0.513276000000	-1.588314000000
H	1.057847000000	-2.825263000000	-1.289246000000
C	-3.880986000000	-0.918716000000	-0.175857000000
C	-1.715954000000	-0.434514000000	-0.382251000000
N	-2.506426000000	0.451628000000	-0.994803000000
N	-2.607425000000	-1.318641000000	0.139195000000
C	-2.293683000000	-2.525618000000	0.896626000000
H	-2.626813000000	-2.409686000000	1.931212000000
H	-2.808556000000	-3.374325000000	0.439391000000
H	-1.217100000000	-2.671123000000	0.867417000000
N	-3.842148000000	0.182019000000	-0.876942000000
C	-5.107203000000	-1.663482000000	0.212297000000
H	-5.125502000000	-2.650487000000	-0.261610000000
H	-5.147926000000	-1.808821000000	1.296282000000
H	-5.987805000000	-1.102127000000	-0.105689000000
C	-2.104626000000	1.643180000000	-1.724969000000
H	-1.136139000000	1.466986000000	-2.191590000000
H	-2.854151000000	1.832334000000	-2.494444000000
H	-2.041576000000	2.500820000000	-1.048160000000

N,N’-dimethylbenzimidazolylidene (**B**)

Carbene neutral singlet

C	0.159633000000	0.699851000000	-0.000035000000
C	0.159629000000	-0.699853000000	-0.000019000000
C	1.346288000000	-1.432187000000	0.000014000000
C	2.534058000000	-0.703609000000	0.000020000000
C	2.534062000000	0.703596000000	0.000004000000
C	1.346296000000	1.432179000000	-0.000024000000

C	-2.013195000000	0.000006000000	0.000023000000
H	1.344583000000	-2.518279000000	0.000022000000
H	3.481768000000	-1.233789000000	0.000041000000
H	3.481775000000	1.233770000000	0.000015000000
H	1.344595000000	2.518271000000	-0.000035000000
N	-1.176746000000	-1.074520000000	-0.000008000000
N	-1.176740000000	1.074526000000	0.000008000000
C	-1.605577000000	-2.461584000000	0.000003000000
H	-1.230484000000	-2.972366000000	0.891634000000
H	-2.695328000000	-2.485176000000	-0.000122000000
H	-1.230282000000	-2.972434000000	-0.891502000000
C	-1.605559000000	2.461594000000	0.000004000000
H	-1.230335000000	2.972419000000	0.891554000000
H	-1.230385000000	2.972394000000	-0.891581000000
H	-2.695310000000	2.485196000000	0.000033000000

TS1 neutral singlet, imaginary frequency = 181.0*i* cm^{-1}

C	1.939665000000	-0.566790000000	-0.491719000000
C	1.982767000000	0.606517000000	0.269098000000
C	3.008253000000	0.854925000000	1.180002000000
C	3.989060000000	-0.126323000000	1.299827000000
C	3.945800000000	-1.307688000000	0.535869000000
C	2.921091000000	-1.550794000000	-0.375444000000
C	0.138637000000	0.690680000000	-1.036389000000
H	3.037697000000	1.767370000000	1.767986000000
H	4.805309000000	0.021824000000	2.000561000000
H	4.729596000000	-2.048597000000	0.661764000000
H	2.886447000000	-2.462275000000	-0.964633000000
N	0.863427000000	1.341311000000	-0.100119000000
N	0.797089000000	-0.466996000000	-1.277448000000
C	-1.918634000000	1.115101000000	-1.329039000000
H	-1.916781000000	0.638466000000	-2.324705000000
O	-2.143386000000	2.336577000000	-1.220405000000
C	-2.316292000000	0.157392000000	-0.228532000000
C	-2.607999000000	-1.174012000000	-0.534111000000
C	-2.424160000000	0.602410000000	1.092308000000
C	-2.992088000000	-2.060293000000	0.473275000000
C	-2.800723000000	-0.282613000000	2.100585000000
C	-3.083911000000	-1.616915000000	1.793112000000
H	-2.538523000000	-1.515184000000	-1.565426000000
H	-2.212524000000	1.645148000000	1.317286000000
H	-3.223513000000	-3.093535000000	0.228517000000
H	-2.878125000000	0.065897000000	3.127129000000
H	-3.381500000000	-2.304911000000	2.579763000000
C	0.370422000000	-1.501857000000	-2.204237000000
H	0.064191000000	-2.397400000000	-1.655169000000

H	-0.468971000000	-1.124988000000	-2.788481000000
H	1.195194000000	-1.752878000000	-2.876652000000
C	0.529404000000	2.638843000000	0.468181000000
H	0.416165000000	2.548239000000	1.552405000000
H	1.327495000000	3.353644000000	0.248125000000
H	-0.406437000000	2.974872000000	0.021021000000

INT1 neutral singlet

C	1.987741000000	-0.800970000000	-0.168278000000
C	2.151901000000	0.547174000000	0.157055000000
C	3.299751000000	1.019306000000	0.793131000000
C	4.277131000000	0.075770000000	1.088095000000
C	4.111870000000	-1.284665000000	0.761707000000
C	2.965134000000	-1.751258000000	0.128927000000
C	0.169470000000	0.314340000000	-0.828742000000
H	3.419793000000	2.068111000000	1.045555000000
H	5.188779000000	0.393542000000	1.584567000000
H	4.899552000000	-1.987957000000	1.013635000000
H	2.837012000000	-2.800453000000	-0.116598000000
N	1.004638000000	1.203633000000	-0.268707000000
N	0.747413000000	-0.902837000000	-0.785214000000
C	-1.236606000000	0.615870000000	-1.408548000000
H	-1.327749000000	-0.123718000000	-2.237682000000
O	-1.397755000000	1.886900000000	-1.788271000000
C	-2.222136000000	0.131719000000	-0.320808000000
C	-3.018484000000	-0.999633000000	-0.506952000000
C	-2.361150000000	0.869317000000	0.861394000000
C	-3.937647000000	-1.394462000000	0.470304000000
C	-3.269410000000	0.476524000000	1.841874000000
C	-4.062281000000	-0.659449000000	1.648075000000
H	-2.926230000000	-1.574540000000	-1.426976000000
H	-1.757588000000	1.764057000000	1.003749000000
H	-4.556623000000	-2.272979000000	0.307777000000
H	-3.364452000000	1.055185000000	2.757062000000
H	-4.774464000000	-0.964097000000	2.410000000000
C	0.168404000000	-2.166372000000	-1.225971000000
H	0.975615000000	-2.806047000000	-1.585619000000
H	-0.347134000000	-2.652030000000	-0.393431000000
H	-0.531550000000	-1.988351000000	-2.040697000000
C	0.796603000000	2.636256000000	-0.058563000000
H	-0.133211000000	2.905945000000	-0.558750000000
H	0.751017000000	2.830480000000	1.016259000000
H	1.643169000000	3.175277000000	-0.491433000000

TS2 neutral singlet, imaginary frequency = 1336.1*i* cm^{-1}

C	-2.562225000000	0.177578000000	-0.632669000000
C	-2.358673000000	-0.478196000000	0.584691000000
C	-3.405783000000	-1.063853000000	1.293021000000
C	-4.673134000000	-0.960857000000	0.727661000000
C	-4.880634000000	-0.301496000000	-0.497518000000
C	-3.830449000000	0.280062000000	-1.202166000000
C	-0.386712000000	0.283156000000	-0.139524000000
H	-3.238610000000	-1.572353000000	2.237491000000
H	-5.521186000000	-1.400516000000	1.243743000000
H	-5.885466000000	-0.242768000000	-0.904527000000
H	-3.993990000000	0.791577000000	-2.145239000000
N	-1.003501000000	-0.384605000000	0.862829000000
N	-1.314576000000	0.618206000000	-1.060917000000
C	1.035484000000	0.648043000000	-0.120057000000
O	1.302966000000	1.719313000000	-1.013418000000
H	1.615441000000	2.490018000000	-0.490467000000
H	1.259834000000	1.133925000000	1.112642000000
O	2.214649000000	3.728958000000	0.682398000000
O	1.616264000000	1.735452000000	2.198163000000
H	2.037392000000	3.042687000000	1.410939000000
H	3.173441000000	3.862581000000	0.651633000000
H	0.813769000000	1.888003000000	2.721735000000
C	2.001005000000	-0.487861000000	-0.287849000000
C	3.367242000000	-0.171672000000	-0.379000000000
C	1.636409000000	-1.842092000000	-0.320186000000
C	4.331110000000	-1.169305000000	-0.493177000000
C	2.604134000000	-2.843429000000	-0.427882000000
C	3.955942000000	-2.515288000000	-0.513785000000
H	3.669252000000	0.872552000000	-0.362048000000
H	0.588917000000	-2.132917000000	-0.278213000000
H	5.381092000000	-0.896298000000	-0.562346000000
H	2.292848000000	-3.884533000000	-0.455697000000
H	4.707234000000	-3.294967000000	-0.602229000000
C	-1.086300000000	1.234980000000	-2.366075000000
H	-1.156832000000	2.321718000000	-2.291736000000
H	-0.102401000000	0.955158000000	-2.732926000000
H	-1.851880000000	0.858232000000	-3.046042000000
C	-0.395343000000	-0.916687000000	2.075097000000
H	-0.978557000000	-0.579670000000	2.935835000000
H	-0.392140000000	-2.009552000000	2.037397000000
H	0.624909000000	-0.546372000000	2.166023000000

BINT neutral singlet

C	-2.024029000000	-0.821897000000	-0.131493000000
C	-2.466932000000	0.494832000000	0.081169000000
C	-3.813549000000	0.777367000000	0.266010000000

C	-4.712087000000	-0.299893000000	0.229335000000
C	-4.271461000000	-1.605274000000	0.006686000000
C	-2.909448000000	-1.888323000000	-0.177197000000
C	-0.213048000000	0.537974000000	-0.147934000000
H	-4.164931000000	1.792566000000	0.421927000000
H	-5.771137000000	-0.107621000000	0.373875000000
H	-4.990051000000	-2.418933000000	-0.021768000000
H	-2.560790000000	-2.903950000000	-0.338720000000
N	-1.347861000000	1.317578000000	0.057980000000
N	-0.643178000000	-0.779629000000	-0.291180000000
C	1.072651000000	1.010950000000	-0.236628000000
O	1.208542000000	2.347743000000	-0.616870000000
H	1.718335000000	2.825305000000	0.060681000000
C	2.298519000000	0.252858000000	-0.018815000000
C	2.349330000000	-0.874711000000	0.829539000000
C	3.510520000000	0.695719000000	-0.588101000000
C	3.544535000000	-1.548188000000	1.057678000000
C	4.706461000000	0.022432000000	-0.347704000000
C	4.734606000000	-1.109000000000	0.469450000000
H	1.445774000000	-1.207089000000	1.334764000000
H	3.504861000000	1.568582000000	-1.234674000000
H	3.550961000000	-2.412506000000	1.717027000000
H	5.622979000000	0.383994000000	-0.807138000000
H	5.667597000000	-1.632847000000	0.655774000000
C	-1.318186000000	2.646309000000	0.644601000000
H	-2.282151000000	2.833507000000	1.121072000000
H	-0.535891000000	2.693507000000	1.408925000000
H	-1.131033000000	3.414462000000	-0.107559000000
C	0.080494000000	-1.815418000000	-1.005395000000
H	0.549713000000	-2.533424000000	-0.325888000000
H	-0.620469000000	-2.345048000000	-1.656483000000
H	0.854907000000	-1.352517000000	-1.621667000000

TS3 neutral singlet, imaginary frequency = 249.0*i* cm^{-1}

C	3.023579000000	0.848649000000	0.378701000000
C	3.281549000000	-0.469109000000	0.000006000000
C	4.497946000000	-1.089999000000	0.276985000000
C	5.445818000000	-0.328004000000	0.955444000000
C	5.188530000000	1.001469000000	1.332707000000
C	3.971994000000	1.617739000000	1.049083000000
C	1.204210000000	0.050368000000	-0.665969000000
H	4.696100000000	-2.115432000000	-0.018862000000
H	6.406875000000	-0.771775000000	1.197211000000
H	5.956066000000	1.561574000000	1.857983000000
H	3.771986000000	2.643930000000	1.341047000000
N	2.144906000000	-0.932884000000	-0.642705000000

N	1.745542000000	1.153503000000	-0.075619000000
C	-0.136740000000	-0.120605000000	-1.204834000000
O	-0.110114000000	-0.639007000000	-2.483662000000
H	-0.602336000000	-1.521028000000	-2.399958000000
C	-0.877072000000	-1.933337000000	-0.286799000000
O	-1.142713000000	-2.578147000000	-1.357125000000
H	0.056581000000	-2.160580000000	0.256523000000
C	-1.971639000000	-1.515514000000	0.630136000000
C	-3.287698000000	-1.387748000000	0.170365000000
C	-1.686477000000	-1.247367000000	1.971946000000
C	-4.297034000000	-0.974595000000	1.037007000000
C	-2.696856000000	-0.844336000000	2.845048000000
C	-4.003804000000	-0.699993000000	2.376952000000
H	-3.505768000000	-1.610378000000	-0.870983000000
H	-0.662399000000	-1.346054000000	2.329981000000
H	-5.314929000000	-0.866918000000	0.670967000000
H	-2.465450000000	-0.638683000000	3.886809000000
H	-4.792795000000	-0.379438000000	3.052065000000
C	-1.202536000000	0.871241000000	-0.944674000000
C	-2.145477000000	1.148513000000	-1.945551000000
C	-1.408121000000	1.442526000000	0.326816000000
C	-3.242219000000	1.976124000000	-1.692683000000
C	-2.494593000000	2.271680000000	0.575715000000
C	-3.425502000000	2.543993000000	-0.433510000000
H	-2.015230000000	0.705321000000	-2.927588000000
H	-0.717904000000	1.218319000000	1.136693000000
H	-3.956930000000	2.172640000000	-2.488119000000
H	-2.627594000000	2.695558000000	1.568276000000
H	-4.280457000000	3.184060000000	-0.233977000000
C	2.101627000000	-2.276937000000	-1.211871000000
H	1.118562000000	-2.494247000000	-1.618236000000
H	2.847338000000	-2.342052000000	-2.009623000000
H	2.345176000000	-2.998487000000	-0.427516000000
C	1.308412000000	2.544326000000	-0.187231000000
H	0.862886000000	2.892069000000	0.747261000000
H	2.189637000000	3.146651000000	-0.418178000000
H	0.592699000000	2.643356000000	-0.999941000000

INT2 neutral singlet

C	-3.279093000000	-0.726495000000	-0.410429000000
C	-3.299007000000	0.392519000000	0.422871000000
C	-4.476387000000	1.090306000000	0.699534000000
C	-5.635653000000	0.611127000000	0.104294000000
C	-5.618952000000	-0.519631000000	-0.735957000000
C	-4.444599000000	-1.209323000000	-1.010221000000
C	-1.192907000000	-0.335735000000	0.285313000000

H	-4.482967000000	1.964551000000	1.342411000000
H	-6.576317000000	1.121149000000	0.287554000000
H	-6.547113000000	-0.860005000000	-1.184334000000
H	-4.443727000000	-2.074759000000	-1.663911000000
N	-1.995175000000	0.594067000000	0.839608000000
N	-1.954478000000	-1.157057000000	-0.466624000000
C	0.331347000000	-0.315148000000	0.619531000000
O	0.455682000000	-0.475117000000	1.951338000000
H	0.626786000000	-2.229177000000	1.562638000000
C	1.113157000000	-1.503044000000	-0.086550000000
O	0.800636000000	-2.646475000000	0.676834000000
H	0.779352000000	-1.640067000000	-1.119466000000
C	2.604868000000	-1.237257000000	-0.114396000000
C	3.390078000000	-1.430687000000	1.026163000000
C	3.213846000000	-0.755348000000	-1.277781000000
C	4.751717000000	-1.125295000000	1.010350000000
C	4.574378000000	-0.446916000000	-1.298003000000
C	5.347542000000	-0.626620000000	-0.149666000000
H	2.928060000000	-1.812662000000	1.931483000000
H	2.614051000000	-0.612968000000	-2.174838000000
H	5.348963000000	-1.275915000000	1.905892000000
H	5.030716000000	-0.071283000000	-2.210030000000
H	6.407637000000	-0.388493000000	-0.161290000000
C	0.864702000000	1.010471000000	0.044527000000
C	0.546372000000	1.426280000000	-1.250984000000
C	1.745761000000	1.775175000000	0.808792000000
C	1.110212000000	2.587921000000	-1.781257000000
C	2.315802000000	2.934305000000	0.281414000000
C	2.000890000000	3.343391000000	-1.016625000000
H	-0.138596000000	0.836847000000	-1.861257000000
H	1.974971000000	1.439659000000	1.816918000000
H	0.855375000000	2.901368000000	-2.790176000000
H	3.005399000000	3.520970000000	0.883003000000
H	2.442784000000	4.246804000000	-1.427824000000
C	-1.603434000000	1.683348000000	1.730573000000
H	-1.473117000000	2.603715000000	1.154518000000
H	-2.400154000000	1.817982000000	2.464937000000
H	-0.682064000000	1.398339000000	2.234473000000
C	-1.562784000000	-2.316049000000	-1.272246000000
H	-1.139863000000	-1.987107000000	-2.223894000000
H	-0.857518000000	-2.929757000000	-0.715786000000
H	-2.462782000000	-2.899306000000	-1.462770000000

TS4 neutral singlet, imaginary frequency = 144.2*i* cm^{-1}

C	-3.388730000000	0.162205000000	0.416012000000
C	-3.284176000000	-0.970567000000	-0.396922000000

C	-4.369930000000	-1.445166000000	-1.133091000000
C	-5.561954000000	-0.734558000000	-1.020249000000
C	-5.666500000000	0.405223000000	-0.201052000000
C	-4.581880000000	0.875077000000	0.533888000000
C	-1.264459000000	-0.611241000000	0.568498000000
H	-4.289569000000	-2.323274000000	-1.766693000000
H	-6.431874000000	-1.065924000000	-1.579548000000
H	-6.615111000000	0.930668000000	-0.142673000000
H	-4.658198000000	1.755294000000	1.165311000000
N	-1.973385000000	-1.415364000000	-0.262542000000
N	-2.136926000000	0.335282000000	0.989726000000
C	0.850284000000	-0.176829000000	0.936992000000
O	1.022315000000	-0.199412000000	2.171104000000
H	1.153787000000	-2.199031000000	1.849561000000
C	1.441438000000	-1.371942000000	0.154582000000
O	1.262408000000	-2.530077000000	0.935232000000
H	0.928649000000	-1.499321000000	-0.802806000000
C	2.909435000000	-1.090022000000	-0.126408000000
C	3.868556000000	-1.216510000000	0.883352000000
C	3.310411000000	-0.664886000000	-1.395835000000
C	5.207015000000	-0.920463000000	0.627046000000
C	4.648979000000	-0.365594000000	-1.654963000000
C	5.600420000000	-0.491752000000	-0.642682000000
H	3.565367000000	-1.548373000000	1.873065000000
H	2.569393000000	-0.570437000000	-2.187473000000
H	5.944611000000	-1.024575000000	1.418313000000
H	4.948523000000	-0.040407000000	-2.647650000000
H	6.643561000000	-0.262605000000	-0.842637000000
C	0.840214000000	1.143905000000	0.194679000000
C	1.383106000000	2.259251000000	0.834940000000
C	0.373369000000	1.267825000000	-1.119073000000
C	1.454601000000	3.488160000000	0.176897000000
C	0.440633000000	2.493558000000	-1.776560000000
C	0.981980000000	3.607990000000	-1.129378000000
H	1.748823000000	2.154659000000	1.852750000000
H	-0.061010000000	0.407849000000	-1.626162000000
H	1.880155000000	4.349872000000	0.684100000000
H	0.067226000000	2.582157000000	-2.793092000000
H	1.033849000000	4.563731000000	-1.643702000000
C	-1.827251000000	1.427455000000	1.899924000000
H	-2.610447000000	1.491026000000	2.660220000000
H	-0.871119000000	1.223391000000	2.380712000000
H	-1.777753000000	2.373352000000	1.350620000000
C	-1.469314000000	-2.602343000000	-0.938019000000
H	-2.242720000000	-3.374503000000	-0.919060000000
H	-1.216410000000	-2.373969000000	-1.977977000000
H	-0.592802000000	-2.965752000000	-0.401635000000

4,5-bis(p-bromophenyl)-1,3-dimethylimidazolylidene (**C**)

Carbene neutral singlet

N	-1.064216000000	3.610946000000	-0.000206000000
C	-0.000050000000	4.456287000000	0.000071000000
C	-0.683691000000	2.273934000000	-0.002571000000
C	0.683707000000	2.273963000000	0.002695000000
N	1.064163000000	3.611004000000	0.000236000000
C	1.611511000000	1.130581000000	-0.022697000000
C	2.651342000000	1.016922000000	0.908786000000
C	1.439980000000	0.116272000000	-0.974004000000
C	3.508536000000	-0.080703000000	0.890001000000
C	2.284901000000	-0.989974000000	-0.998627000000
C	3.313665000000	-1.073270000000	-0.065373000000
H	2.786921000000	1.778601000000	1.671276000000
H	0.641836000000	0.193719000000	-1.707583000000
H	4.308883000000	-0.160218000000	1.618444000000
H	2.144996000000	-1.768512000000	-1.741406000000
C	-1.611471000000	1.130537000000	0.022784000000
C	-2.651375000000	1.016984000000	-0.908626000000
C	-1.439893000000	0.116153000000	0.974004000000
C	-3.508577000000	-0.080635000000	-0.889884000000
C	-2.284818000000	-0.990092000000	0.998577000000
C	-3.313639000000	-1.073298000000	0.065379000000
H	-2.787024000000	1.778768000000	-1.671003000000
H	-0.641703000000	0.193533000000	1.707539000000
H	-4.308984000000	-0.160069000000	-1.618269000000
H	-2.144871000000	-1.768697000000	1.741279000000
C	2.444989000000	4.074459000000	-0.035955000000
H	2.438506000000	5.122373000000	-0.334915000000
H	2.914319000000	3.984294000000	0.946758000000
C	-2.445082000000	4.074294000000	0.035763000000
H	-2.914262000000	3.984031000000	-0.947015000000
H	-3.015598000000	3.494109000000	0.764651000000
H	-2.438738000000	5.122221000000	0.334678000000
Br	4.477537000000	-2.574228000000	-0.098859000000
Br	-4.477525000000	-2.574246000000	0.098811000000
H	3.015455000000	3.494298000000	-0.764901000000

TS1 neutral singlet, imaginary frequency = 177.3*i* cm^{-1}

C	4.332799000000	-2.395577000000	-0.008583000000
O	4.100850000000	-3.097906000000	0.993776000000
C	5.332002000000	-1.267221000000	0.037639000000
C	5.802625000000	-0.706381000000	-1.151530000000

C	5.799087000000	-0.786104000000	1.261208000000
C	6.712622000000	0.348499000000	-1.120953000000
H	5.436115000000	-1.087299000000	-2.104022000000
C	6.708381000000	0.271649000000	1.295996000000
C	7.161777000000	0.844862000000	0.105848000000
H	7.071544000000	0.785037000000	-2.049233000000
H	7.064693000000	0.650423000000	2.250334000000
H	7.867998000000	1.670359000000	0.133507000000
H	5.434456000000	-1.239423000000	2.179330000000
H	4.257007000000	-2.834847000000	-1.020613000000
N	2.167008000000	0.026805000000	-0.243666000000
C	2.568816000000	-1.261272000000	-0.346339000000
C	0.782104000000	0.121752000000	-0.143358000000
C	0.309764000000	-1.161415000000	-0.170841000000
N	1.425642000000	-1.980302000000	-0.298004000000
C	-1.081975000000	-1.641710000000	-0.132259000000
C	-1.479306000000	-2.640690000000	0.764554000000
C	-2.036676000000	-1.077222000000	-0.988023000000
C	-2.802009000000	-3.074396000000	0.805941000000
C	-3.363902000000	-1.494952000000	-0.949735000000
C	-3.730398000000	-2.492388000000	-0.051394000000
H	-0.758834000000	-3.076439000000	1.451085000000
H	-1.740042000000	-0.307657000000	-1.696178000000
H	-3.101156000000	-3.849194000000	1.504441000000
H	-4.095229000000	-1.053764000000	-1.619371000000
C	0.026211000000	1.381381000000	-0.041301000000
C	0.233214000000	2.420057000000	-0.957557000000
C	-0.952767000000	1.533213000000	0.948913000000
C	-0.519265000000	3.589317000000	-0.890139000000
C	-1.718631000000	2.693774000000	1.021135000000
C	-1.492282000000	3.709587000000	0.097305000000
H	0.976041000000	2.314258000000	-1.743725000000
H	-1.118515000000	0.738813000000	1.671930000000
H	-0.354682000000	4.385937000000	-1.608235000000
H	-2.476208000000	2.801163000000	1.790572000000
C	1.371796000000	-3.433011000000	-0.432721000000
H	0.517964000000	-3.703383000000	-1.057098000000
H	2.287582000000	-3.772905000000	-0.912083000000
C	3.073435000000	1.173293000000	-0.223560000000
H	3.283490000000	1.514223000000	-1.240669000000
H	2.612071000000	1.983556000000	0.342531000000
H	4.001857000000	0.884706000000	0.266922000000
Br	-5.537451000000	-3.074130000000	0.004273000000
Br	-2.537555000000	5.292220000000	0.177886000000
H	1.279209000000	-3.909254000000	0.545049000000

INT1 neutral singlet

C	-4.119202000000	-1.281508000000	-1.207948000000
O	-4.456988000000	-0.719686000000	-2.377583000000
C	-4.994611000000	-0.885409000000	0.006111000000
C	-4.727972000000	-1.374748000000	1.290537000000
C	-6.087541000000	-0.042050000000	-0.183383000000
C	-5.538213000000	-1.021073000000	2.368706000000
H	-3.877814000000	-2.038911000000	1.449738000000
C	-6.904245000000	0.314946000000	0.893406000000
C	-6.631439000000	-0.172016000000	2.172003000000
H	-5.319880000000	-1.406284000000	3.361416000000
H	-7.753859000000	0.974423000000	0.734262000000
H	-7.264519000000	0.105038000000	3.010573000000
H	-6.277054000000	0.325074000000	-1.188633000000
H	-4.133939000000	-2.394929000000	-1.218428000000
N	-1.642067000000	-1.785364000000	-0.642485000000
C	-2.664632000000	-0.937956000000	-0.832867000000
C	-0.472765000000	-1.062799000000	-0.435648000000
C	-0.817009000000	0.260982000000	-0.489478000000
N	-2.179959000000	0.307169000000	-0.737399000000
C	0.037341000000	1.451309000000	-0.347808000000
C	-0.298616000000	2.473497000000	0.547611000000
C	1.219958000000	1.551307000000	-1.090528000000
C	0.529299000000	3.582571000000	0.699317000000
C	2.059094000000	2.651925000000	-0.942034000000
C	1.701216000000	3.656216000000	-0.047485000000
H	-1.203351000000	2.402162000000	1.144866000000
H	1.485967000000	0.767365000000	-1.794493000000
H	0.264022000000	4.369880000000	1.397141000000
H	2.973081000000	2.724134000000	-1.522338000000
C	0.848911000000	-1.667598000000	-0.205689000000
C	1.362082000000	-2.628043000000	-1.085518000000
C	1.624419000000	-1.250149000000	0.882443000000
C	2.627841000000	-3.170603000000	-0.881400000000
C	2.894895000000	-1.779174000000	1.091931000000
C	3.380317000000	-2.736042000000	0.205687000000
H	0.779444000000	-2.946891000000	-1.945976000000
H	1.231990000000	-0.510048000000	1.574793000000
H	3.021010000000	-3.913067000000	-1.567904000000
H	3.490125000000	-1.452126000000	1.938177000000
C	-2.987624000000	1.514056000000	-0.917171000000
H	-3.824116000000	1.242119000000	-1.562988000000
H	-3.341950000000	1.873751000000	0.051871000000
C	-1.758260000000	-3.244121000000	-0.590908000000
H	-1.754201000000	-3.658589000000	-1.601228000000
H	-0.913949000000	-3.637508000000	-0.025865000000

H	-2.680536000000	-3.513636000000	-0.078198000000
Br	2.838877000000	5.162814000000	0.157591000000
Br	5.109212000000	-3.468720000000	0.485793000000
H	-2.372946000000	2.278482000000	-1.394690000000

TS2 neutral singlet, imaginary frequency = 1086.1*i* cm^{-1}

C	3.956548000000	-0.235374000000	0.612022000000
C	4.698351000000	0.314438000000	-0.547776000000
C	5.962852000000	0.905491000000	-0.373101000000
C	4.214330000000	0.179689000000	-1.864638000000
C	6.710132000000	1.338800000000	-1.468655000000
H	6.351318000000	1.023889000000	0.634022000000
C	4.964803000000	0.611363000000	-2.955497000000
C	6.220801000000	1.195216000000	-2.768046000000
H	7.684186000000	1.793740000000	-1.304134000000
H	4.563521000000	0.494055000000	-3.959210000000
H	6.804850000000	1.531582000000	-3.619959000000
H	3.238501000000	-0.273465000000	-2.037642000000
H	4.520591000000	-1.553757000000	0.757387000000
O	4.301336000000	0.435571000000	1.830503000000
H	4.371216000000	-0.248878000000	2.527412000000
O	4.459993000000	-1.832912000000	3.477579000000
O	5.087796000000	-2.564023000000	1.033641000000
H	4.787257000000	-2.270919000000	2.636091000000
H	5.180319000000	-1.891520000000	4.122580000000
H	6.024876000000	-2.415026000000	0.831704000000
N	1.643028000000	-1.204029000000	0.238376000000
C	2.481856000000	-0.169166000000	0.421677000000
C	0.342982000000	-0.741357000000	0.130704000000
C	0.398787000000	0.623534000000	0.244903000000
N	1.731711000000	0.949777000000	0.415619000000
C	-0.709711000000	1.593627000000	0.251261000000
C	-0.700564000000	2.722489000000	-0.576360000000
C	-1.814489000000	1.359560000000	1.078984000000
C	-1.774750000000	3.609078000000	-0.575038000000
C	-2.896760000000	2.233473000000	1.082077000000
C	-2.862525000000	3.350994000000	0.253217000000
H	0.138350000000	2.907814000000	-1.241472000000
H	-1.829177000000	0.489677000000	1.730209000000
H	-1.762766000000	4.480814000000	-1.220932000000
H	-3.749966000000	2.043864000000	1.725016000000
C	-0.833553000000	-1.605375000000	-0.063879000000
C	-1.080374000000	-2.685034000000	0.791792000000
C	-1.748386000000	-1.312722000000	-1.082154000000
C	-2.222578000000	-3.464916000000	0.634722000000
C	-2.898049000000	-2.080470000000	-1.244061000000

C	-3.120703000000	-3.148350000000	-0.380003000000
H	-0.391232000000	-2.910137000000	1.601093000000
H	-1.560870000000	-0.479952000000	-1.754990000000
H	-2.412063000000	-4.296846000000	1.305391000000
H	-3.603993000000	-1.847867000000	-2.034909000000
C	2.272400000000	2.300581000000	0.557739000000
H	3.239731000000	2.228915000000	1.051626000000
H	2.381288000000	2.762274000000	-0.426421000000
C	2.047058000000	-2.604903000000	0.112084000000
H	1.401668000000	-3.084860000000	-0.624646000000
H	3.083184000000	-2.648316000000	-0.216899000000
H	1.950762000000	-3.109538000000	1.075993000000
Br	-4.339172000000	4.543295000000	0.250766000000
Br	-4.691378000000	-4.197327000000	-0.584251000000
H	1.590775000000	2.892254000000	1.171047000000

BINT neutral singlet

C	-3.829170000000	-1.681277000000	-0.376859000000
O	-3.956605000000	-2.949897000000	-0.955329000000
C	-5.041885000000	-0.994823000000	0.016829000000
C	-5.050607000000	0.071032000000	0.949306000000
C	-6.295673000000	-1.439415000000	-0.463203000000
C	-6.238426000000	0.678625000000	1.338946000000
H	-4.115582000000	0.402268000000	1.394569000000
C	-7.481538000000	-0.829439000000	-0.060965000000
C	-7.468489000000	0.240322000000	0.836367000000
H	-6.205553000000	1.493181000000	2.058626000000
H	-8.426386000000	-1.193431000000	-0.457574000000
H	-8.394204000000	0.715340000000	1.147492000000
H	-6.329400000000	-2.263215000000	-1.170149000000
H	-4.365619000000	-3.558254000000	-0.315429000000
N	-2.121554000000	0.122914000000	-0.306014000000
C	-2.536867000000	-1.196384000000	-0.282070000000
C	-0.722670000000	0.158949000000	-0.200113000000
C	-0.278904000000	-1.125097000000	-0.131740000000
N	-1.394130000000	-1.967180000000	-0.192957000000
C	1.091411000000	-1.639589000000	-0.013821000000
C	1.522073000000	-2.695289000000	-0.829137000000
C	1.990384000000	-1.078522000000	0.902540000000
C	2.825804000000	-3.174996000000	-0.743708000000
C	3.298805000000	-1.544917000000	0.992181000000
C	3.702236000000	-2.589107000000	0.165110000000
H	0.837297000000	-3.141650000000	-1.546026000000
H	1.665318000000	-0.274983000000	1.557786000000
H	3.151200000000	-3.989136000000	-1.383056000000
H	3.987824000000	-1.103725000000	1.705122000000

C	0.025561000000	1.420674000000	-0.188621000000
C	-0.433301000000	2.504885000000	0.573326000000
C	1.208601000000	1.563897000000	-0.926840000000
C	0.276910000000	3.701213000000	0.611484000000
C	1.932317000000	2.751964000000	-0.888297000000
C	1.457647000000	3.809457000000	-0.117532000000
H	-1.347288000000	2.412181000000	1.154519000000
H	1.565495000000	0.744275000000	-1.544328000000
H	-0.085857000000	4.531955000000	1.208182000000
H	2.847388000000	2.851620000000	-1.463149000000
C	-1.419784000000	-3.334001000000	0.308066000000
H	-2.220740000000	-3.426159000000	1.048443000000
H	-1.590505000000	-4.052254000000	-0.496156000000
C	-2.893658000000	1.182171000000	-0.938419000000
H	-3.406430000000	1.813483000000	-0.207022000000
H	-2.225081000000	1.801479000000	-1.539631000000
H	-3.640697000000	0.723852000000	-1.592023000000
Br	5.483850000000	-3.237050000000	0.286114000000
Br	2.435720000000	5.437386000000	-0.069430000000
H	-0.468167000000	-3.551561000000	0.794322000000

TS3 neutral singlet, imaginary frequency = 191.2*i* cm^{-1}

C	0.387204000000	0.487140000000	-0.617802000000
C	0.572746000000	-0.862758000000	-0.625530000000
C	-1.604184000000	-0.474853000000	-1.030607000000
N	-0.661877000000	-1.444572000000	-0.884245000000
N	-0.955734000000	0.716996000000	-0.904295000000
C	-3.018523000000	-0.710468000000	-1.240855000000
O	-3.264138000000	-1.626434000000	-2.244150000000
H	-3.721305000000	-2.397326000000	-1.787836000000
C	-3.612371000000	-2.155165000000	0.414821000000
O	-4.037059000000	-3.074741000000	-0.347819000000
H	-2.585832000000	-2.208361000000	0.817575000000
C	-4.538080000000	-1.387305000000	1.280691000000
C	-5.906749000000	-1.321428000000	0.989949000000
C	-4.042759000000	-0.724054000000	2.406875000000
C	-6.762008000000	-0.586632000000	1.806817000000
C	-4.900176000000	-0.000680000000	3.235468000000
C	-6.260592000000	0.075511000000	2.932396000000
H	-6.286727000000	-1.845902000000	0.116955000000
H	-2.977859000000	-0.773392000000	2.630310000000
H	-7.821639000000	-0.529861000000	1.571024000000
H	-4.507843000000	0.506464000000	4.112989000000
H	-6.929452000000	0.646078000000	3.571181000000
C	-4.015006000000	0.358703000000	-1.085787000000
C	-5.152516000000	0.378209000000	-1.911490000000

C	-3.957062000000	1.301350000000	-0.037013000000
C	-6.173872000000	1.309724000000	-1.712271000000
C	-4.970672000000	2.230745000000	0.155828000000
C	-6.092853000000	2.244396000000	-0.681545000000
H	-5.231516000000	-0.348251000000	-2.714277000000
H	-3.116317000000	1.289697000000	0.652900000000
H	-7.039570000000	1.300061000000	-2.370243000000
H	-4.895539000000	2.940234000000	0.976771000000
H	-6.888107000000	2.967866000000	-0.525440000000
C	-0.849169000000	-2.890492000000	-1.003088000000
H	-1.899395000000	-3.147104000000	-0.906808000000
H	-0.493397000000	-3.226959000000	-1.980030000000
H	-0.278459000000	-3.382903000000	-0.213542000000
C	-1.420411000000	2.003210000000	-1.430968000000
H	-1.795077000000	2.653675000000	-0.639362000000
H	-0.576207000000	2.482907000000	-1.928716000000
H	-2.207232000000	1.825827000000	-2.162149000000
C	1.362317000000	1.562526000000	-0.391292000000
C	1.053271000000	2.646529000000	0.440191000000
C	2.623742000000	1.504520000000	-0.997237000000
C	1.984804000000	3.656226000000	0.665937000000
C	3.565615000000	2.503323000000	-0.771330000000
C	3.233900000000	3.570778000000	0.058009000000
H	0.082899000000	2.701501000000	0.926682000000
H	2.871840000000	0.678718000000	-1.658498000000
H	1.736318000000	4.491817000000	1.312312000000
H	4.539951000000	2.450175000000	-1.246050000000
C	1.803718000000	-1.621951000000	-0.342727000000
C	2.498296000000	-1.377786000000	0.847785000000
C	2.318695000000	-2.547213000000	-1.258411000000
C	3.689708000000	-2.042387000000	1.124594000000
C	3.504899000000	-3.224230000000	-0.988672000000
C	4.177818000000	-2.961602000000	0.200967000000
H	2.104832000000	-0.663849000000	1.566551000000
H	1.806088000000	-2.730697000000	-2.198377000000
H	4.220692000000	-1.847658000000	2.050773000000
H	3.900361000000	-3.938090000000	-1.703778000000
Br	5.794918000000	-3.881072000000	0.571644000000
Br	4.511453000000	4.942342000000	0.353567000000

INT2 neutral singlet

C	3.196136000000	-0.856627000000	-0.214704000000
O	3.420498000000	-2.120878000000	-0.617561000000
C	3.718144000000	-0.603039000000	1.218688000000
C	4.402373000000	0.538680000000	1.647035000000
C	3.478347000000	-1.621089000000	2.151986000000

C	4.836842000000	0.659207000000	2.970744000000
H	4.619583000000	1.346343000000	0.954701000000
C	3.900191000000	-1.502316000000	3.473854000000
C	4.586599000000	-0.358070000000	3.888971000000
H	5.375740000000	1.551711000000	3.277502000000
H	3.700665000000	-2.304069000000	4.179968000000
H	4.925263000000	-0.264070000000	4.917041000000
H	2.965398000000	-2.519871000000	1.818614000000
C	8.093642000000	0.511602000000	-1.342422000000
C	7.270429000000	1.635969000000	-1.396963000000
C	5.882542000000	1.483707000000	-1.385221000000
C	5.296313000000	0.215988000000	-1.316091000000
C	6.131490000000	-0.908680000000	-1.273309000000
C	7.518208000000	-0.760155000000	-1.281768000000
H	9.174430000000	0.623603000000	-1.350407000000
H	7.705688000000	2.630401000000	-1.449581000000
H	5.243794000000	2.364922000000	-1.420993000000
H	5.677211000000	-1.893397000000	-1.217132000000
H	8.154279000000	-1.640744000000	-1.241327000000
C	3.781967000000	0.094180000000	-1.340855000000
O	3.350203000000	-0.499392000000	-2.554383000000
H	3.370010000000	1.104572000000	-1.311253000000
H	3.334590000000	-1.455747000000	-2.291047000000
N	1.017859000000	0.624873000000	-0.062782000000
C	1.641166000000	-0.571774000000	-0.148462000000
C	-0.356514000000	0.442376000000	-0.057361000000
C	-0.572081000000	-0.902086000000	-0.115008000000
N	0.673395000000	-1.509882000000	-0.171433000000
C	-1.859316000000	-1.620182000000	-0.161579000000
C	-2.200403000000	-2.567109000000	0.810984000000
C	-2.780494000000	-1.306884000000	-1.167177000000
C	-3.439988000000	-3.199826000000	0.777481000000
C	-4.026245000000	-1.928010000000	-1.207546000000
C	-4.339103000000	-2.870037000000	-0.232827000000
H	-1.504888000000	-2.803812000000	1.611134000000
H	-2.523443000000	-0.572419000000	-1.925830000000
H	-3.700122000000	-3.930773000000	1.535968000000
H	-4.735231000000	-1.680008000000	-1.990558000000
C	-1.345314000000	1.531577000000	0.004727000000
C	-1.304754000000	2.597392000000	-0.902223000000
C	-2.370675000000	1.478249000000	0.956042000000
C	-2.269068000000	3.600485000000	-0.858133000000
C	-3.344985000000	2.471279000000	1.004431000000
C	-3.280085000000	3.522705000000	0.095485000000
H	-0.526136000000	2.641201000000	-1.659231000000
H	-2.406953000000	0.657817000000	1.667881000000
H	-2.233931000000	4.423090000000	-1.564990000000

H	-4.137346000000	2.423923000000	1.744158000000
C	0.806149000000	-2.973623000000	-0.227792000000
H	0.057569000000	-3.353814000000	-0.924699000000
H	1.816251000000	-3.201099000000	-0.554074000000
C	1.621916000000	1.943831000000	0.143300000000
H	1.736016000000	2.468579000000	-0.806834000000
H	0.964233000000	2.514531000000	0.799643000000
H	2.585144000000	1.834859000000	0.631971000000
Br	-6.034079000000	-3.725338000000	-0.278870000000
Br	-4.603233000000	4.882779000000	0.156914000000
H	0.623115000000	-3.385265000000	0.767165000000

TS4 neutral singlet, imaginary frequency = 129.5*i* cm^{-1}

C	3.553519000000	-0.864740000000	0.268912000000
O	3.503646000000	-1.949237000000	0.897916000000
C	3.490245000000	0.421166000000	1.068539000000
C	4.251770000000	1.550298000000	0.759596000000
C	2.629757000000	0.464110000000	2.172480000000
C	4.160366000000	2.702128000000	1.545579000000
H	4.914632000000	1.552703000000	-0.099889000000
C	2.520178000000	1.616766000000	2.943586000000
C	3.292357000000	2.741699000000	2.634007000000
H	4.763026000000	3.571058000000	1.295983000000
H	1.837043000000	1.640533000000	3.788500000000
H	3.214381000000	3.641060000000	3.238772000000
H	2.033310000000	-0.414295000000	2.408905000000
C	8.631643000000	-0.418245000000	-0.361110000000
C	7.990019000000	0.290447000000	-1.376877000000
C	6.617982000000	0.132958000000	-1.576677000000
C	5.869901000000	-0.728381000000	-0.768240000000
C	6.523167000000	-1.442014000000	0.243767000000
C	7.894260000000	-1.286325000000	0.446586000000
H	9.698970000000	-0.295143000000	-0.198547000000
H	8.556476000000	0.966201000000	-2.012183000000
H	6.118132000000	0.692337000000	-2.365421000000
H	5.953358000000	-2.113850000000	0.880469000000
H	8.388246000000	-1.840070000000	1.240584000000
C	4.378372000000	-0.895800000000	-1.035948000000
O	4.133441000000	-2.140293000000	-1.666018000000
H	4.050951000000	-0.103993000000	-1.715847000000
H	3.932963000000	-2.752564000000	-0.930795000000
N	0.925599000000	0.533611000000	-0.668123000000
C	1.611518000000	-0.629889000000	-0.578956000000
C	-0.439994000000	0.338709000000	-0.512864000000
C	-0.614504000000	-1.007286000000	-0.347768000000
N	0.656643000000	-1.569560000000	-0.388889000000

C	-1.865530000000	-1.755689000000	-0.137412000000
C	-2.758838000000	-1.339229000000	0.857328000000
C	-2.204866000000	-2.850398000000	-0.942089000000
C	-3.973468000000	-1.992789000000	1.044162000000
C	-3.413132000000	-3.518407000000	-0.759683000000
C	-4.286096000000	-3.077242000000	0.230119000000
H	-2.503484000000	-0.495574000000	1.493353000000
H	-1.532746000000	-3.177617000000	-1.730823000000
H	-4.660171000000	-1.659028000000	1.815499000000
H	-3.670760000000	-4.362609000000	-1.391077000000
C	-1.440506000000	1.418888000000	-0.515554000000
C	-2.594549000000	1.316536000000	-1.302113000000
C	-1.274790000000	2.538499000000	0.309333000000
C	-3.569824000000	2.309775000000	-1.265612000000
C	-2.236760000000	3.543666000000	0.345614000000
C	-3.376913000000	3.413939000000	-0.441126000000
H	-2.733062000000	0.454363000000	-1.949637000000
H	-0.398647000000	2.620381000000	0.947743000000
H	-4.463415000000	2.221908000000	-1.875416000000
H	-2.101932000000	4.406234000000	0.990188000000
C	0.928612000000	-2.997923000000	-0.256786000000
H	1.927235000000	-3.116469000000	0.159625000000
H	0.198542000000	-3.442836000000	0.421688000000
C	1.541558000000	1.821020000000	-0.965433000000
H	2.501507000000	1.639233000000	-1.447977000000
H	0.897390000000	2.377657000000	-1.649450000000
H	1.695786000000	2.402119000000	-0.052202000000
Br	-5.944997000000	-3.969745000000	0.469137000000
Br	-4.702611000000	4.773923000000	-0.378809000000
H	0.863458000000	-3.487554000000	-1.231818000000

N,N’-dimethylimidazolyl-idene (**D**)

Carbene neutral singlet

C	-0.678418000000	1.196649000000	0.000029000000
C	0.678445000000	1.196629000000	-0.000016000000
C	-0.000036000000	-0.984736000000	-0.000029000000
N	-1.061002000000	-0.132883000000	0.000030000000
H	-1.393021000000	2.007422000000	0.000046000000
H	1.393026000000	2.007428000000	-0.000084000000
N	1.061021000000	-0.132874000000	-0.000068000000
C	-2.453715000000	-0.552225000000	-0.000001000000
H	-2.960773000000	-0.173874000000	-0.891411000000
H	-2.486060000000	-1.641792000000	0.000046000000

H	-2.960836000000	-0.173788000000	0.891336000000
C	2.453704000000	-0.552241000000	0.000038000000
H	2.960708000000	-0.174066000000	0.891559000000
H	2.485998000000	-1.641810000000	-0.000180000000
H	2.960948000000	-0.173678000000	-0.891177000000

TS1 neutral singlet, imaginary frequency = 178.9*i* cm^{-1}

C	-0.344167000000	-0.529240000000	1.753552000000
O	-0.360021000000	-1.702844000000	2.159624000000
C	-1.318275000000	-0.059003000000	0.699423000000
C	-1.504884000000	1.308367000000	0.473662000000
C	-2.068663000000	-0.985433000000	-0.027637000000
C	-2.420076000000	1.746268000000	-0.481693000000
H	-0.925038000000	2.029227000000	1.048712000000
C	-2.982632000000	-0.549504000000	-0.987640000000
C	-3.158358000000	0.816120000000	-1.218354000000
H	-2.561325000000	2.810300000000	-0.651943000000
H	-3.562324000000	-1.274757000000	-1.552791000000
H	-3.871834000000	1.156598000000	-1.963814000000
H	-1.933323000000	-2.045693000000	0.169840000000
H	0.003838000000	0.283958000000	2.412979000000
C	2.699936000000	0.845820000000	-1.082695000000
C	2.446927000000	-0.406262000000	-1.543035000000
C	1.363091000000	-0.177784000000	0.433282000000
N	2.027626000000	0.959401000000	0.121695000000
H	3.295787000000	1.650424000000	-1.489490000000
H	2.772548000000	-0.920848000000	-2.435931000000
N	1.630705000000	-1.006079000000	-0.600974000000
C	2.037960000000	2.165679000000	0.936385000000
H	1.548258000000	2.984179000000	0.402474000000
H	1.503517000000	1.963634000000	1.864830000000
H	3.068468000000	2.447237000000	1.165752000000
C	1.092196000000	-2.353677000000	-0.726972000000
H	1.909579000000	-3.066611000000	-0.861016000000
H	0.544903000000	-2.588565000000	0.186808000000
H	0.420468000000	-2.407686000000	-1.588120000000

INT1 neutral singlet

C	3.060096000000	-0.352763000000	0.921209000000
C	2.586361000000	0.860061000000	1.309211000000
C	1.225815000000	0.073919000000	-0.263819000000
N	2.202096000000	-0.822747000000	-0.054050000000
H	3.923644000000	-0.918784000000	1.236364000000
H	2.949576000000	1.570649000000	2.036513000000
N	1.453816000000	1.103844000000	0.562688000000

C	2.354200000000	-2.100710000000	-0.747546000000
H	1.495337000000	-2.742231000000	-0.544877000000
H	2.450460000000	-1.931033000000	-1.821098000000
H	3.260161000000	-2.574900000000	-0.370797000000
C	0.095323000000	0.009402000000	-1.302937000000
O	0.123395000000	1.072994000000	-2.117882000000
C	-1.219753000000	-0.191321000000	-0.508715000000
C	-1.392595000000	-1.277340000000	0.357851000000
C	-2.265330000000	0.714655000000	-0.674748000000
C	-2.589825000000	-1.450548000000	1.051162000000
H	-0.583475000000	-1.996390000000	0.489843000000
C	-3.468570000000	0.545628000000	0.016491000000
C	-3.633569000000	-0.535564000000	0.882494000000
H	-2.711476000000	-2.297523000000	1.721525000000
H	-4.277795000000	1.258709000000	-0.120616000000
H	-4.568101000000	-0.668974000000	1.420702000000
H	-2.110830000000	1.547280000000	-1.355990000000
H	0.267090000000	-0.968424000000	-1.812660000000
C	0.601169000000	2.283395000000	0.686429000000
H	-0.161009000000	2.108774000000	1.450095000000
H	1.227680000000	3.127722000000	0.977413000000
H	0.140260000000	2.460621000000	-0.286323000000

TS2 neutral singlet, imaginary frequency = 1299.5*i* cm^{-1}

C	-2.998604000000	-1.587395000000	-0.488993000000
C	-2.695525000000	-1.748910000000	0.823108000000
C	-1.170254000000	-0.381114000000	-0.065656000000
N	-1.570091000000	-0.990058000000	1.071491000000
N	-2.042029000000	-0.749861000000	-1.027006000000
C	-0.032615000000	0.549606000000	-0.182548000000
O	-0.225323000000	1.450367000000	-1.269083000000
H	-0.562966000000	2.295158000000	-0.904997000000
H	0.037441000000	1.361358000000	0.947425000000
O	-1.136134000000	3.730898000000	0.091127000000
O	0.094075000000	2.224872000000	1.829933000000
H	-0.656104000000	3.308846000000	0.869947000000
H	-0.678327000000	4.562473000000	-0.101023000000
H	1.031774000000	2.444022000000	1.947181000000
C	1.312769000000	-0.090597000000	-0.224825000000
C	2.423425000000	0.704268000000	-0.567002000000
C	1.552735000000	-1.430817000000	0.124954000000
C	3.714645000000	0.183272000000	-0.551719000000
C	2.848408000000	-1.949028000000	0.146696000000
C	3.939180000000	-1.147272000000	-0.188344000000
H	2.257604000000	1.740204000000	-0.850754000000
H	0.722994000000	-2.092238000000	0.364801000000

H	4.552917000000	0.820209000000	-0.823392000000
H	3.001590000000	-2.991212000000	0.415812000000
H	4.946906000000	-1.552753000000	-0.174764000000
C	-1.973366000000	-0.402943000000	-2.445462000000
H	-0.946711000000	-0.498143000000	-2.796992000000
H	-2.614435000000	-1.103299000000	-2.981876000000
H	-2.317327000000	0.619057000000	-2.603466000000
C	-0.927301000000	-0.883692000000	2.377096000000
H	-1.696548000000	-1.002919000000	3.141604000000
H	-0.173935000000	-1.666827000000	2.494406000000
H	-0.465570000000	0.101149000000	2.471950000000
H	-3.799217000000	-1.989888000000	-1.091445000000
H	-3.177173000000	-2.317133000000	1.604553000000

BINT neutral singlet

C	2.747402000000	-1.626905000000	0.042816000000
C	3.402487000000	-0.489072000000	-0.268176000000
C	1.243013000000	0.058228000000	0.097824000000
N	2.484431000000	0.552717000000	-0.231178000000
N	1.416035000000	-1.296087000000	0.286919000000
C	0.078740000000	0.807949000000	0.259446000000
O	0.269702000000	2.123789000000	0.709273000000
H	-0.053202000000	2.745390000000	0.034032000000
C	-1.272750000000	0.358042000000	0.045995000000
C	-1.594085000000	-0.758187000000	-0.769957000000
C	-2.363187000000	1.090514000000	0.579936000000
C	-2.911852000000	-1.143021000000	-0.984617000000
C	-3.679940000000	0.701350000000	0.350420000000
C	-3.973999000000	-0.424548000000	-0.423245000000
H	-0.796225000000	-1.302729000000	-1.269007000000
H	-2.161040000000	1.962971000000	1.194501000000
H	-3.114794000000	-2.003901000000	-1.617654000000
H	-4.487641000000	1.284911000000	0.786569000000
H	-5.002364000000	-0.725713000000	-0.599411000000
C	0.503062000000	-2.161145000000	1.008008000000
H	-0.194959000000	-2.673972000000	0.340035000000
H	1.089815000000	-2.903629000000	1.551926000000
H	-0.069668000000	-1.559662000000	1.720366000000
C	2.725139000000	1.875375000000	-0.777961000000
H	3.712563000000	1.875521000000	-1.242137000000
H	1.971991000000	2.100581000000	-1.540869000000
H	2.686576000000	2.640309000000	-0.000757000000
H	3.096850000000	-2.643890000000	0.138923000000
H	4.437041000000	-0.314394000000	-0.523820000000

TS3 neutral singlet, imaginary frequency = 142.5*i* cm^{-1}

C	-3.577308000000	0.854774000000	-1.545548000000
C	-3.973685000000	-0.329164000000	-1.029792000000
C	-2.064613000000	0.249331000000	0.001556000000
N	-3.040328000000	-0.700041000000	-0.081458000000
N	-2.415440000000	1.223272000000	-0.886593000000
C	-0.916650000000	0.173556000000	0.870301000000
O	-1.241600000000	-0.219558000000	2.155942000000
H	-0.794492000000	-1.102023000000	2.295097000000
C	0.008857000000	-1.958643000000	0.365200000000
O	-0.062673000000	-2.394157000000	1.543883000000
H	-0.806256000000	-2.161430000000	-0.350973000000
C	1.302404000000	-1.634962000000	-0.273499000000
C	2.454665000000	-1.441055000000	0.499427000000
C	1.379709000000	-1.526560000000	-1.665654000000
C	3.665173000000	-1.133954000000	-0.115386000000
C	2.594800000000	-1.233235000000	-2.283641000000
C	3.738468000000	-1.032102000000	-1.508681000000
H	2.385264000000	-1.530712000000	1.580449000000
H	0.480244000000	-1.670850000000	-2.262897000000
H	4.555800000000	-0.974285000000	0.487087000000
H	2.649746000000	-1.156957000000	-3.366267000000
H	4.685585000000	-0.798468000000	-1.987655000000
C	0.258224000000	1.030389000000	0.733419000000
C	0.988069000000	1.403741000000	1.879166000000
C	0.796460000000	1.393846000000	-0.521329000000
C	2.175601000000	2.129915000000	1.776159000000
C	1.971755000000	2.126480000000	-0.619688000000
C	2.676909000000	2.504187000000	0.530040000000
H	0.612102000000	1.116736000000	2.856264000000
H	0.298596000000	1.068359000000	-1.431664000000
H	2.712268000000	2.403350000000	2.681733000000
H	2.356806000000	2.386110000000	-1.603476000000
H	3.602463000000	3.067494000000	0.450363000000
C	-3.230716000000	-1.876578000000	0.763449000000
H	-2.279605000000	-2.271072000000	1.110487000000
H	-3.844598000000	-1.612224000000	1.628562000000
H	-3.745379000000	-2.632586000000	0.167931000000
C	-1.912535000000	2.592663000000	-0.957771000000
H	-1.159345000000	2.703146000000	-1.739930000000
H	-2.762269000000	3.239974000000	-1.180015000000
H	-1.489060000000	2.878552000000	0.004465000000
H	-4.017634000000	1.488987000000	-2.300210000000
H	-4.829202000000	-0.950775000000	-1.247987000000

INT2 neutral singlet

C	-0.476437000000	-0.320932000000	0.451935000000
O	-0.503795000000	-0.769460000000	1.720464000000
C	-0.029559000000	1.156042000000	0.360693000000
C	0.787507000000	1.692976000000	-0.638806000000
C	-0.479677000000	2.007931000000	1.376968000000
C	1.150312000000	3.042266000000	-0.620286000000
H	1.150817000000	1.067360000000	-1.448487000000
C	-0.132238000000	3.357649000000	1.394509000000
C	0.690920000000	3.880509000000	0.394564000000
H	1.793611000000	3.435068000000	-1.403336000000
H	-0.496531000000	4.000339000000	2.191829000000
H	0.972644000000	4.929823000000	0.408336000000
H	-1.097190000000	1.586860000000	2.165942000000
C	4.682730000000	-0.874152000000	-0.007781000000
C	4.097690000000	-0.984114000000	-1.268888000000
C	2.712936000000	-1.124035000000	-1.384903000000
C	1.895228000000	-1.154650000000	-0.251554000000
C	2.492956000000	-1.055399000000	1.012280000000
C	3.874637000000	-0.911312000000	1.131810000000
H	5.759363000000	-0.763000000000	0.088388000000
H	4.716538000000	-0.961651000000	-2.162046000000
H	2.259479000000	-1.201838000000	-2.371883000000
H	1.856395000000	-1.075968000000	1.892546000000
H	4.324673000000	-0.826891000000	2.117700000000
C	0.396533000000	-1.336845000000	-0.406374000000
O	0.002903000000	-2.610738000000	0.075432000000
H	0.153669000000	-1.296117000000	-1.473688000000
H	-0.233263000000	-2.374596000000	1.013531000000
C	-4.101719000000	-0.832148000000	-0.306228000000
C	-3.714609000000	-0.244828000000	-1.463897000000
C	-1.922921000000	-0.399030000000	-0.140327000000
N	-2.987191000000	-0.920927000000	0.500652000000
H	-5.063217000000	-1.198797000000	0.019124000000
H	-4.264267000000	0.013207000000	-2.356642000000
N	-2.367045000000	0.014459000000	-1.346562000000
C	-3.074342000000	-1.532592000000	1.834476000000
H	-2.464024000000	-2.432683000000	1.874986000000
H	-2.732935000000	-0.831320000000	2.590085000000
H	-4.124168000000	-1.787267000000	1.986731000000
C	-1.626262000000	0.710332000000	-2.397717000000
H	-1.496047000000	1.760342000000	-2.130382000000
H	-0.656260000000	0.244157000000	-2.559251000000
H	-2.214609000000	0.633827000000	-3.312126000000

TS4 neutral singlet, imaginary frequency = 160.0*i* cm^{-1}

C	0.024105000000	-0.573544000000	-0.521038000000
O	0.116668000000	-1.211039000000	-1.591629000000
C	0.180893000000	0.931094000000	-0.557895000000
C	-0.360579000000	1.778630000000	0.412776000000
C	0.896390000000	1.487394000000	-1.624895000000
C	-0.189484000000	3.161112000000	0.317196000000
H	-0.915816000000	1.372792000000	1.253368000000
C	1.079031000000	2.864481000000	-1.714555000000
C	0.533150000000	3.707208000000	-0.742309000000
H	-0.619972000000	3.810048000000	1.075106000000
H	1.642536000000	3.284078000000	-2.543748000000
H	0.669854000000	4.782833000000	-0.813011000000
H	1.309780000000	0.822797000000	-2.379096000000
C	-5.040943000000	-0.064416000000	0.016265000000
C	-4.423981000000	0.071765000000	1.259517000000
C	-3.084515000000	-0.288240000000	1.415649000000
C	-2.346141000000	-0.785911000000	0.338912000000
C	-2.974893000000	-0.924983000000	-0.904680000000
C	-4.312276000000	-0.565583000000	-1.064816000000
H	-6.083271000000	0.215101000000	-0.110725000000
H	-4.983566000000	0.455753000000	2.108425000000
H	-2.605212000000	-0.178906000000	2.386988000000
H	-2.412880000000	-1.314068000000	-1.750551000000
H	-4.787492000000	-0.676331000000	-2.035909000000
C	-0.896591000000	-1.208203000000	0.545279000000
O	-0.772094000000	-2.612214000000	0.430283000000
H	-0.586617000000	-0.919113000000	1.552582000000
H	-0.468930000000	-2.752118000000	-0.489764000000
C	3.947513000000	-0.072774000000	1.165174000000
C	4.177393000000	-0.882297000000	0.100660000000
C	1.939254000000	-0.846541000000	0.450210000000
N	2.579071000000	-0.071896000000	1.360089000000
H	4.621060000000	0.481290000000	1.803195000000
H	5.095041000000	-1.186291000000	-0.382246000000
N	2.941251000000	-1.343622000000	-0.313630000000
C	1.934365000000	0.681100000000	2.425437000000
H	2.463942000000	0.501484000000	3.363995000000
H	1.948443000000	1.750466000000	2.197891000000
H	0.903971000000	0.341687000000	2.524725000000
C	2.780149000000	-2.268444000000	-1.430657000000
H	1.910962000000	-2.899413000000	-1.255349000000
H	2.644849000000	-1.721196000000	-2.366084000000
H	3.677433000000	-2.887334000000	-1.491617000000

4,5-di(2,2’-bithiophene)-1,3-dimethylimidazolylidene (**E**)

Carbene neutral singlet

C	0.653564000000	2.696908000000	-0.203907000000
C	-0.653733000000	2.696896000000	0.203896000000
N	-1.016731000000	4.032581000000	0.315606000000
N	1.016535000000	4.032599000000	-0.315626000000
C	-1.554197000000	1.572850000000	0.434084000000
C	-2.337930000000	1.305976000000	1.527397000000
S	-1.752203000000	0.350972000000	-0.786435000000
C	-3.081141000000	0.099900000000	1.398715000000
H	-2.360136000000	1.940586000000	2.406958000000
C	-2.861431000000	-0.544103000000	0.204630000000
H	-3.731124000000	-0.290221000000	2.175484000000
C	1.554056000000	1.572883000000	-0.434099000000
C	2.337669000000	1.305954000000	-1.527483000000
S	1.752263000000	0.351118000000	0.786500000000
C	3.080952000000	0.099924000000	-1.398789000000
H	2.359740000000	1.940494000000	-2.407098000000
C	2.861418000000	-0.543987000000	-0.204621000000
H	3.730860000000	-0.290232000000	-2.175602000000
C	3.431098000000	-1.797151000000	0.271302000000
C	2.914723000000	-2.681264000000	1.187052000000
S	4.969272000000	-2.349352000000	-0.320977000000
C	3.757456000000	-3.811677000000	1.405138000000
H	1.954981000000	-2.541118000000	1.674670000000
C	4.896994000000	-3.770377000000	0.653307000000
H	3.519270000000	-4.622044000000	2.084971000000
H	5.703298000000	-4.492762000000	0.613989000000
C	-3.430986000000	-1.797337000000	-0.271260000000
C	-2.914435000000	-2.681505000000	-1.186857000000
S	-4.969224000000	-2.349554000000	0.320837000000
C	-3.757081000000	-3.811979000000	-1.404964000000
H	-1.954629000000	-2.541355000000	-1.674347000000
C	-4.896730000000	-3.770668000000	-0.653302000000
H	-3.518756000000	-4.622396000000	-2.084689000000
H	-5.703003000000	-4.493090000000	-0.614036000000
C	-0.000106000000	4.877726000000	-0.000016000000
C	-2.343216000000	4.481499000000	0.714704000000
H	-2.403674000000	5.552923000000	0.525763000000
H	-3.105052000000	3.963590000000	0.126997000000
H	-2.512291000000	4.289911000000	1.777109000000
C	2.343013000000	4.481531000000	-0.714735000000
H	2.403445000000	5.552965000000	-0.525841000000
H	3.104857000000	3.963665000000	-0.127000000000
H	2.512098000000	4.289899000000	-1.777129000000

TS1 neutral singlet, imaginary frequency = 251.7*i* cm^{-1}

C	4.822372000000	-2.008852000000	-0.151208000000
O	4.364609000000	-2.792508000000	0.710474000000
C	5.695136000000	-0.846820000000	0.255877000000
C	6.586257000000	-0.289163000000	-0.662840000000
C	5.628880000000	-0.336329000000	1.552759000000
C	7.390433000000	0.789951000000	-0.296807000000
H	6.638503000000	-0.694467000000	-1.672488000000
C	6.427547000000	0.745721000000	1.920998000000
C	7.305975000000	1.314224000000	0.995172000000
H	8.081939000000	1.221418000000	-1.015550000000
H	6.364331000000	1.149503000000	2.928173000000
H	7.926915000000	2.158804000000	1.281110000000
H	4.936996000000	-0.785503000000	2.261169000000
H	5.091546000000	-2.390126000000	-1.153584000000
C	0.910255000000	-1.093457000000	-0.729214000000
C	1.277594000000	0.177323000000	-0.374973000000
N	2.665779000000	0.212167000000	-0.447910000000
N	2.086039000000	-1.774993000000	-0.999229000000
C	0.438197000000	1.315432000000	-0.024816000000
C	0.575090000000	2.197478000000	1.017292000000
S	-0.957423000000	1.700696000000	-0.987697000000
C	-0.460066000000	3.171314000000	1.060952000000
H	1.375577000000	2.131673000000	1.746686000000
C	-1.379261000000	3.026564000000	0.049515000000
H	-0.539283000000	3.929081000000	1.834055000000
C	-0.418896000000	-1.696293000000	-0.776896000000
C	-1.070911000000	-2.271880000000	-1.836153000000
S	-1.399197000000	-1.734823000000	0.657353000000
C	-2.377393000000	-2.725288000000	-1.502812000000
H	-0.637470000000	-2.345026000000	-2.828120000000
C	-2.710049000000	-2.494601000000	-0.189199000000
H	-3.055795000000	-3.180450000000	-2.217673000000
C	-3.949838000000	-2.814312000000	0.504945000000
C	-4.457090000000	-2.257111000000	1.653499000000
S	-5.005542000000	-4.056040000000	-0.098115000000
C	-5.703504000000	-2.829656000000	2.045719000000
H	-3.965990000000	-1.452591000000	2.192305000000
C	-6.123382000000	-3.807978000000	1.189900000000
H	-6.263742000000	-2.521480000000	2.921460000000
H	-7.028556000000	-4.400863000000	1.238638000000
C	-2.581153000000	3.807856000000	-0.207814000000
C	-3.724208000000	3.425870000000	-0.867503000000
S	-2.711079000000	5.446927000000	0.355180000000
C	-4.710721000000	4.454954000000	-0.911661000000
H	-3.866377000000	2.435209000000	-1.288732000000

C	-4.304020000000	5.599035000000	-0.285665000000
H	-5.681890000000	4.342493000000	-1.380679000000
H	-4.846775000000	6.528389000000	-0.163783000000
C	3.169236000000	-0.988914000000	-0.819530000000
C	3.452535000000	1.424610000000	-0.237116000000
H	2.954702000000	2.259721000000	-0.734502000000
H	3.552353000000	1.640571000000	0.828770000000
H	4.437769000000	1.279221000000	-0.677273000000
C	2.134766000000	-3.180427000000	-1.382086000000
H	1.622029000000	-3.784315000000	-0.629533000000
H	1.656180000000	-3.318233000000	-2.353745000000
H	3.176591000000	-3.486872000000	-1.440059000000

INT1 neutral singlet

C	-4.670121000000	-1.399808000000	-1.008627000000
O	-5.074365000000	-1.073682000000	-2.241453000000
C	-5.393386000000	-0.669890000000	0.154281000000
C	-5.092298000000	-0.951807000000	1.492198000000
C	-6.383333000000	0.267162000000	-0.134186000000
C	-5.765193000000	-0.300399000000	2.524962000000
H	-4.325946000000	-1.691000000000	1.728236000000
C	-7.062710000000	0.922127000000	0.897093000000
C	-6.754547000000	0.641955000000	2.228549000000
H	-5.522306000000	-0.527566000000	3.559778000000
H	-7.834053000000	1.650974000000	0.660914000000
H	-7.281754000000	1.150076000000	3.031380000000
H	-6.607142000000	0.465213000000	-1.179173000000
H	-4.770653000000	-2.479932000000	-0.757881000000
C	-1.238381000000	-0.001443000000	-0.758738000000
C	-0.994898000000	-1.278792000000	-0.327611000000
N	-2.210577000000	-1.950819000000	-0.375952000000
N	-2.589000000000	0.070148000000	-1.052247000000
C	0.264175000000	-1.880281000000	0.088946000000
C	0.514211000000	-2.673063000000	1.180579000000
S	1.711043000000	-1.609743000000	-0.834177000000
C	1.880120000000	-3.050278000000	1.289587000000
H	-0.250781000000	-2.955184000000	1.896275000000
C	2.661345000000	-2.541525000000	0.279466000000
H	2.273208000000	-3.650627000000	2.103762000000
C	-0.316758000000	1.126253000000	-0.867364000000
C	0.109276000000	1.777147000000	-1.995052000000
S	0.428796000000	1.780864000000	0.557219000000
C	1.060300000000	2.797775000000	-1.718135000000
H	-0.228404000000	1.512346000000	-2.991696000000
C	1.351027000000	2.912726000000	-0.379415000000
H	1.533897000000	3.402433000000	-2.484848000000

C	2.274922000000	3.829201000000	0.275568000000
C	2.953393000000	3.660138000000	1.457764000000
S	2.640867000000	5.373365000000	-0.432863000000
C	3.777932000000	4.776003000000	1.789135000000
H	2.883797000000	2.760112000000	2.060914000000
C	3.713651000000	5.771832000000	0.856144000000
H	4.396583000000	4.828713000000	2.677970000000
H	4.235597000000	6.720782000000	0.849183000000
C	4.093410000000	-2.699635000000	0.068252000000
C	4.956215000000	-1.869723000000	-0.605461000000
S	4.933310000000	-4.084485000000	0.699110000000
C	6.300238000000	-2.347548000000	-0.605381000000
H	4.646793000000	-0.937906000000	-1.068887000000
C	6.437604000000	-3.528616000000	0.066975000000
H	7.127073000000	-1.829478000000	-1.078069000000
H	7.337523000000	-4.109114000000	0.229251000000
C	-3.168345000000	-1.111461000000	-0.805591000000
C	-2.397593000000	-3.364926000000	-0.049960000000
H	-1.462595000000	-3.887826000000	-0.250488000000
H	-2.668540000000	-3.478406000000	1.001624000000
H	-3.179614000000	-3.777724000000	-0.684842000000
C	-3.299186000000	1.278052000000	-1.472311000000
H	-2.699404000000	1.798203000000	-2.219451000000
H	-4.245817000000	0.957368000000	-1.907996000000
H	-3.456176000000	1.925615000000	-0.605550000000

TS2 neutral singlet, imaginary frequency = 1319.0*i* cm^{-1}

C	4.352049000000	-0.265851000000	-0.584525000000
C	5.194232000000	-0.256918000000	0.651516000000
C	6.575636000000	-0.482996000000	0.514583000000
C	4.700407000000	0.017583000000	1.937650000000
C	7.426542000000	-0.434296000000	1.615594000000
H	6.977168000000	-0.703002000000	-0.471120000000
C	5.555433000000	0.072479000000	3.039847000000
C	6.923347000000	-0.151061000000	2.888205000000
H	8.489673000000	-0.616199000000	1.479592000000
H	5.143095000000	0.279991000000	4.023986000000
H	7.586774000000	-0.112444000000	3.747420000000
H	3.635540000000	0.171330000000	2.097695000000
H	4.631738000000	0.899103000000	-1.247459000000
O	4.721344000000	-1.301673000000	-1.486522000000
H	5.106253000000	-0.894310000000	-2.292029000000
O	5.862746000000	0.064320000000	-3.640823000000
O	5.031404000000	1.854124000000	-1.969526000000
H	5.613533000000	0.882169000000	-3.098003000000
H	4.245023000000	2.316098000000	-2.301294000000

H	6.830187000000	0.015946000000	-3.642172000000
C	0.731839000000	-0.837223000000	-0.366765000000
C	0.822465000000	0.466289000000	0.038507000000
N	2.169236000000	0.794840000000	0.031277000000
N	2.029175000000	-1.281035000000	-0.589491000000
C	-0.239238000000	1.413655000000	0.358892000000
C	-0.430467000000	2.131414000000	1.511015000000
S	-1.482560000000	1.749991000000	-0.805695000000
C	-1.601381000000	2.937540000000	1.471628000000
H	0.232436000000	2.062740000000	2.367233000000
C	-2.290899000000	2.827410000000	0.287460000000
H	-1.937145000000	3.550933000000	2.301684000000
C	-0.451363000000	-1.671560000000	-0.523777000000
C	-0.795363000000	-2.469340000000	-1.584937000000
S	-1.644573000000	-1.750976000000	0.736013000000
C	-2.028582000000	-3.148714000000	-1.388733000000
H	-0.184441000000	-2.560849000000	-2.477104000000
C	-2.613525000000	-2.864227000000	-0.177701000000
H	-2.460113000000	-3.831720000000	-2.113331000000
C	-3.872520000000	-3.358112000000	0.362465000000
C	-4.256217000000	-3.466957000000	1.676902000000
S	-5.137261000000	-3.903810000000	-0.698027000000
C	-5.570606000000	-3.999430000000	1.829951000000
H	-3.615089000000	-3.195297000000	2.509874000000
C	-6.162992000000	-4.287277000000	0.633195000000
H	-6.048346000000	-4.167057000000	2.788722000000
H	-7.147102000000	-4.702512000000	0.453524000000
C	-3.530962000000	3.480876000000	-0.107997000000
C	-4.474826000000	3.050885000000	-1.008468000000
S	-3.982594000000	5.012174000000	0.578415000000
C	-5.570335000000	3.955128000000	-1.138899000000
H	-4.401518000000	2.109441000000	-1.544167000000
C	-5.443026000000	5.053498000000	-0.336670000000
H	-6.418188000000	3.788518000000	-1.793840000000
C	2.895228000000	-0.273597000000	-0.360246000000
C	2.691909000000	2.116874000000	0.366086000000
H	2.113738000000	2.870186000000	-0.173292000000
H	2.609367000000	2.286951000000	1.441675000000
H	3.737111000000	2.172320000000	0.065379000000
C	2.393822000000	-2.675163000000	-0.849785000000
H	1.610018000000	-3.306618000000	-0.430871000000
H	2.487239000000	-2.852315000000	-1.921764000000
H	3.341316000000	-2.887470000000	-0.360462000000
H	-6.122931000000	5.889734000000	-0.228644000000

BINT neutral singlet

C	-2.363589000000	-3.524910000000	-0.211067000000
O	-1.736988000000	-4.726009000000	-0.558753000000
C	-3.800560000000	-3.547348000000	-0.010866000000
C	-4.481863000000	-2.558511000000	0.737165000000
C	-4.564941000000	-4.632709000000	-0.494697000000
C	-5.853839000000	-2.633724000000	0.948585000000
H	-3.920840000000	-1.740463000000	1.182388000000
C	-5.938039000000	-4.704399000000	-0.271611000000
C	-6.599528000000	-3.703964000000	0.443414000000
H	-6.344408000000	-1.857063000000	1.530254000000
H	-6.496693000000	-5.550137000000	-0.665219000000
H	-7.670261000000	-3.761361000000	0.615613000000
H	-4.071309000000	-5.416381000000	-1.061999000000
H	-1.870556000000	-5.378158000000	0.150986000000
C	-0.716599000000	-0.311548000000	-0.211987000000
C	0.316386000000	-1.143744000000	0.086704000000
N	-0.177513000000	-2.451041000000	0.114468000000
N	-1.871378000000	-1.093205000000	-0.359466000000
C	1.707616000000	-0.809920000000	0.350586000000
C	2.193585000000	0.137554000000	1.213543000000
S	3.000128000000	-1.573638000000	-0.531860000000
C	3.609701000000	0.264136000000	1.162313000000
H	1.550901000000	0.729113000000	1.857530000000
C	4.196660000000	-0.596233000000	0.266749000000
H	4.170830000000	0.971897000000	1.764302000000
C	-0.707003000000	1.129736000000	-0.395592000000
C	0.191677000000	1.881475000000	-1.108835000000
S	-1.878334000000	2.145190000000	0.398525000000
C	-0.048197000000	3.279692000000	-1.008986000000
H	1.001793000000	1.441046000000	-1.681117000000
C	-1.136438000000	3.587727000000	-0.229152000000
H	0.566569000000	4.030001000000	-1.496203000000
C	-1.695932000000	4.896298000000	0.077408000000
C	-2.467069000000	5.269927000000	1.151303000000
S	-1.424594000000	6.245425000000	-0.985688000000
C	-2.833144000000	6.648571000000	1.121232000000
H	-2.747753000000	4.589275000000	1.949131000000
C	-2.334254000000	7.300904000000	0.029874000000
H	-3.432886000000	7.132446000000	1.883993000000
H	-2.447271000000	8.343662000000	-0.240401000000
C	5.609272000000	-0.772206000000	-0.038739000000
C	6.180209000000	-1.273371000000	-1.183232000000
S	6.830321000000	-0.335640000000	1.119756000000
C	7.605553000000	-1.298872000000	-1.129420000000
H	5.602678000000	-1.594621000000	-2.044585000000

C	8.095103000000	-0.815335000000	0.050422000000
H	8.235765000000	-1.653049000000	-1.937543000000
H	9.128595000000	-0.712410000000	0.357485000000
C	-1.537761000000	-2.421459000000	-0.141424000000
C	0.454754000000	-3.542127000000	0.842987000000
H	1.301156000000	-3.145245000000	1.406224000000
H	-0.267011000000	-3.964222000000	1.549113000000
H	0.800047000000	-4.327780000000	0.168268000000
C	-2.993396000000	-0.683062000000	-1.191348000000
H	-2.668004000000	0.121321000000	-1.854887000000
H	-3.309257000000	-1.537602000000	-1.795834000000
H	-3.844452000000	-0.339317000000	-0.596206000000

TS3 neutral singlet, imaginary frequency = 185.8*i* cm^{-1}

C	-2.131714000000	-0.050440000000	-1.166235000000
N	-1.222395000000	-1.047852000000	-1.314904000000
N	-1.432202000000	1.060252000000	-0.793868000000
C	-3.564119000000	-0.187099000000	-1.344248000000
O	-3.903353000000	-0.785500000000	-2.540988000000
H	-4.366552000000	-1.640720000000	-2.282456000000
C	-4.112027000000	-2.013199000000	-0.116685000000
O	-4.626040000000	-2.677164000000	-1.066885000000
H	-3.066661000000	-2.206308000000	0.180300000000
C	-4.942839000000	-1.485273000000	0.991726000000
C	-6.323389000000	-1.308448000000	0.835976000000
C	-4.342773000000	-1.160085000000	2.211678000000
C	-7.086476000000	-0.796973000000	1.882417000000
C	-5.107520000000	-0.663237000000	3.266634000000
C	-6.480516000000	-0.473789000000	3.100998000000
H	-6.785643000000	-1.570035000000	-0.112423000000
H	-3.268231000000	-1.294471000000	2.330107000000
H	-8.155857000000	-0.650728000000	1.752751000000
H	-4.633279000000	-0.419548000000	4.213632000000
H	-7.078695000000	-0.079549000000	3.918197000000
C	-4.498271000000	0.830544000000	-0.841813000000
C	-5.683529000000	1.101123000000	-1.546681000000
C	-4.328271000000	1.457000000000	0.411266000000
C	-6.646492000000	1.972024000000	-1.031950000000
C	-5.283839000000	2.327936000000	0.918271000000
C	-6.456215000000	2.594069000000	0.201004000000
H	-5.846428000000	0.619496000000	-2.506021000000
H	-3.444381000000	1.239121000000	1.006839000000
H	-7.552018000000	2.163413000000	-1.602876000000
H	-5.123990000000	2.789208000000	1.890246000000
H	-7.205730000000	3.270528000000	0.602105000000
C	-1.445708000000	-2.410970000000	-1.795224000000

H	-2.509198000000	-2.623368000000	-1.842800000000
H	-1.012678000000	-2.512868000000	-2.793557000000
H	-0.959015000000	-3.111011000000	-1.112585000000
C	-1.879091000000	2.444735000000	-0.970993000000
H	-2.200387000000	2.888943000000	-0.027947000000
H	-1.041206000000	3.012213000000	-1.378888000000
H	-2.703290000000	2.459611000000	-1.682921000000
C	-0.088816000000	0.731480000000	-0.638603000000
C	0.920957000000	1.674780000000	-0.187601000000
C	0.790803000000	2.666029000000	0.754020000000
S	2.528416000000	1.646189000000	-0.847639000000
C	1.986427000000	3.408047000000	0.946838000000
H	-0.130928000000	2.852880000000	1.295291000000
C	3.021203000000	2.979060000000	0.150326000000
H	2.073056000000	4.234114000000	1.645540000000
C	0.042379000000	-0.580603000000	-0.989055000000
C	1.237826000000	-1.421719000000	-0.985407000000
C	1.948932000000	-1.895207000000	-2.056031000000
S	1.959986000000	-1.912160000000	0.516062000000
C	3.086885000000	-2.657013000000	-1.671472000000
H	1.670450000000	-1.692213000000	-3.085046000000
C	3.231732000000	-2.757824000000	-0.308202000000
H	3.767798000000	-3.119614000000	-2.378814000000
C	4.387128000000	3.478943000000	0.085137000000
C	5.293821000000	3.365176000000	-0.941000000000
S	5.079893000000	4.339568000000	1.427655000000
C	6.546888000000	3.979213000000	-0.646695000000
H	5.070879000000	2.873044000000	-1.882928000000
C	6.573016000000	4.550085000000	0.594095000000
H	7.387033000000	3.999768000000	-1.331866000000
H	7.385592000000	5.082879000000	1.072636000000
C	4.270698000000	-3.444714000000	0.447361000000
C	4.215705000000	-3.928237000000	1.731920000000
S	5.831306000000	-3.741444000000	-0.258352000000
C	5.432170000000	-4.546826000000	2.145472000000
H	3.329386000000	-3.864148000000	2.355754000000
C	6.389251000000	-4.525758000000	1.170672000000
H	5.582253000000	-4.994393000000	3.121655000000
H	7.396147000000	-4.923156000000	1.209346000000

INT2 neutral singlet

C	3.663491000000	-0.878887000000	0.012009000000
O	3.943649000000	-2.191845000000	-0.066222000000
C	4.174252000000	-0.279472000000	1.342370000000
C	4.972969000000	0.858841000000	1.475003000000
C	3.811002000000	-0.972016000000	2.505376000000

C	5.406033000000	1.288094000000	2.733272000000
H	5.256547000000	1.439301000000	0.603008000000
C	4.227824000000	-0.542641000000	3.762980000000
C	5.035775000000	0.591398000000	3.881500000000
H	6.030735000000	2.174119000000	2.809746000000
H	3.927692000000	-1.093737000000	4.650383000000
H	5.370206000000	0.927317000000	4.859182000000
H	3.199629000000	-1.866511000000	2.410783000000
C	8.454310000000	0.413458000000	-1.634825000000
C	7.567157000000	1.434816000000	-1.973643000000
C	6.190987000000	1.229282000000	-1.857172000000
C	5.681361000000	0.008985000000	-1.402622000000
C	6.579387000000	-1.016003000000	-1.075511000000
C	7.954473000000	-0.811910000000	-1.186551000000
H	9.526291000000	0.568634000000	-1.721306000000
H	7.943734000000	2.390918000000	-2.327456000000
H	5.502744000000	2.032906000000	-2.113670000000
H	6.182638000000	-1.962115000000	-0.718920000000
H	8.640638000000	-1.612327000000	-0.921807000000
C	4.178160000000	-0.186242000000	-1.320581000000
O	3.743680000000	-1.065236000000	-2.348391000000
H	3.695901000000	0.781742000000	-1.498696000000
H	3.808846000000	-1.938938000000	-1.886754000000
C	0.095373000000	0.339329000000	0.135184000000
C	-0.093342000000	-0.961305000000	-0.239812000000
N	1.161119000000	-1.545839000000	-0.319612000000
N	1.463087000000	0.519391000000	0.261614000000
C	-1.347820000000	-1.666740000000	-0.480011000000
C	-1.757194000000	-2.330953000000	-1.606785000000
S	-2.570236000000	-1.706696000000	0.752561000000
C	-3.073248000000	-2.856859000000	-1.491158000000
H	-1.143659000000	-2.417288000000	-2.497361000000
C	-3.654911000000	-2.588435000000	-0.274749000000
H	-3.580387000000	-3.387512000000	-2.290565000000
C	-0.902694000000	1.380733000000	0.348217000000
C	-1.101382000000	2.165483000000	1.454659000000
S	-2.065563000000	1.735204000000	-0.891659000000
C	-2.210803000000	3.043762000000	1.317209000000
H	-0.484659000000	2.098022000000	2.344990000000
C	-2.847825000000	2.920533000000	0.104911000000
H	-2.539813000000	3.721211000000	2.098660000000
C	-4.016315000000	3.636643000000	-0.387021000000
C	-4.896704000000	3.261751000000	-1.372747000000
S	-4.453676000000	5.181851000000	0.277581000000
C	-5.930511000000	4.220419000000	-1.588567000000
H	-4.821386000000	2.323890000000	-1.914578000000
C	-5.821674000000	5.304254000000	-0.764292000000

H	-6.722802000000	4.102393000000	-2.319256000000
H	-6.465453000000	6.173498000000	-0.707619000000
C	-4.982725000000	-2.953592000000	0.199933000000
C	-5.757617000000	-2.324067000000	1.143408000000
S	-5.792828000000	-4.356311000000	-0.429871000000
C	-7.012241000000	-2.969778000000	1.352471000000
H	-5.452577000000	-1.417669000000	1.657239000000
C	-7.170883000000	-4.075788000000	0.566614000000
H	-7.764400000000	-2.619693000000	2.050477000000
H	-8.019578000000	-4.746623000000	0.514161000000
C	2.104588000000	-0.637107000000	-0.011646000000
C	1.329227000000	-2.955430000000	-0.700396000000
H	0.529674000000	-3.525587000000	-0.225447000000
H	1.247734000000	-3.043846000000	-1.786250000000
H	2.309705000000	-3.275127000000	-0.361905000000
C	2.062627000000	1.804296000000	0.625234000000
H	1.369712000000	2.590568000000	0.326438000000
H	2.233309000000	1.848131000000	1.703123000000
H	3.001134000000	1.942216000000	0.094934000000

TS4 neutral singlet, imaginary frequency = 119.6*i* cm^{-1}

C	4.090336000000	-0.827688000000	0.125521000000
O	4.083309000000	-2.057788000000	0.360414000000
C	4.153575000000	0.124953000000	1.299771000000
C	4.846988000000	1.336956000000	1.259553000000
C	3.501328000000	-0.246123000000	2.481133000000
C	4.886960000000	2.165722000000	2.383362000000
H	5.353739000000	1.654784000000	0.353064000000
C	3.526051000000	0.585063000000	3.597128000000
C	4.224166000000	1.795734000000	3.551734000000
H	5.434252000000	3.103384000000	2.339648000000
H	3.003368000000	0.291063000000	4.503385000000
H	4.248896000000	2.443876000000	4.423379000000
H	2.964588000000	-1.191259000000	2.509949000000
C	9.062911000000	-0.158145000000	-1.001621000000
C	8.322002000000	0.850279000000	-1.617775000000
C	6.929755000000	0.764799000000	-1.662105000000
C	6.260291000000	-0.323631000000	-1.095286000000
C	7.011658000000	-1.333645000000	-0.482451000000
C	8.402958000000	-1.250306000000	-0.434853000000
H	10.146940000000	-0.094608000000	-0.963239000000
H	8.825768000000	1.703047000000	-2.064997000000
H	6.354842000000	1.555558000000	-2.140889000000
H	6.504707000000	-2.185327000000	-0.036319000000
H	8.972705000000	-2.039669000000	0.048341000000
C	4.742706000000	-0.411760000000	-1.209980000000

O	4.385966000000	-1.379525000000	-2.180705000000
H	4.355590000000	0.555100000000	-1.544193000000
H	4.271940000000	-2.207709000000	-1.674030000000
C	-0.167649000000	-0.796725000000	-0.450808000000
C	-0.024091000000	0.534966000000	-0.170413000000
N	1.343986000000	0.778484000000	-0.163257000000
N	1.117713000000	-1.307191000000	-0.584039000000
C	-1.048622000000	1.546987000000	0.048788000000
C	-1.082617000000	2.543324000000	0.992248000000
S	-2.462886000000	1.598401000000	-0.961802000000
C	-2.258306000000	3.338976000000	0.919154000000
H	-0.303075000000	2.684485000000	1.733340000000
C	-3.114105000000	2.945268000000	-0.081480000000
H	-2.475211000000	4.153420000000	1.603012000000
C	-1.384082000000	-1.594989000000	-0.583022000000
C	-1.881056000000	-2.203180000000	-1.705891000000
S	-2.412186000000	-1.877723000000	0.788143000000
C	-3.097845000000	-2.900223000000	-1.468303000000
H	-1.390336000000	-2.144505000000	-2.672141000000
C	-3.518559000000	-2.818175000000	-0.162127000000
H	-3.634543000000	-3.451369000000	-2.234072000000
C	-4.709451000000	-3.397231000000	0.445390000000
C	-4.930137000000	-3.716778000000	1.763027000000
S	-6.101391000000	-3.780486000000	-0.524013000000
C	-6.221495000000	-4.278759000000	1.990295000000
H	-4.188054000000	-3.576127000000	2.542859000000
C	-6.958676000000	-4.379713000000	0.844758000000
H	-7.960630000000	-4.773037000000	0.723790000000
C	-4.409985000000	3.503224000000	-0.442137000000
C	-5.460727000000	2.886883000000	-1.077031000000
S	-4.797081000000	5.157994000000	-0.071451000000
C	-6.583973000000	3.747238000000	-1.257248000000
H	-5.441819000000	1.846301000000	-1.386341000000
C	-6.371645000000	4.999862000000	-0.755758000000
H	-7.510369000000	3.441754000000	-1.730991000000
H	-7.048296000000	5.845779000000	-0.750643000000
C	2.054094000000	-0.348844000000	-0.411603000000
C	1.944702000000	2.094189000000	0.022315000000
H	1.302952000000	2.848033000000	-0.437749000000
H	2.070313000000	2.317446000000	1.085694000000
H	2.915776000000	2.099849000000	-0.470852000000
C	1.396752000000	-2.699124000000	-0.923809000000
H	1.355001000000	-2.836648000000	-2.007533000000
H	2.386462000000	-2.951363000000	-0.548000000000
H	0.648950000000	-3.337606000000	-0.449320000000
H	-6.579112000000	-4.602487000000	2.961360000000

4,5-bis(p-chlorophenyl)-1,3-dimethylimidazolylidene

Carbene neutral singlet

N	-1.063950000000	3.020555000000	0.022021000000
C	-0.000048000000	3.865922000000	0.000058000000
C	-0.683649000000	1.683346000000	0.011526000000
C	0.683656000000	1.683371000000	-0.011436000000
N	1.063893000000	3.020604000000	-0.021991000000
C	1.612185000000	0.540715000000	-0.049715000000
C	2.667542000000	0.433010000000	0.865097000000
C	1.426285000000	-0.478481000000	-0.993290000000
C	3.525231000000	-0.663739000000	0.838741000000
C	2.270389000000	-1.585200000000	-1.025560000000
C	3.313748000000	-1.661416000000	-0.107822000000
H	2.814142000000	1.199244000000	1.620897000000
H	0.615986000000	-0.404814000000	-1.713760000000
H	4.339706000000	-0.744219000000	1.551734000000
H	2.122437000000	-2.371299000000	-1.759314000000
C	-1.612154000000	0.540673000000	0.049772000000
C	-2.667577000000	0.433055000000	-0.864972000000
C	-1.426205000000	-0.478590000000	0.993265000000
C	-3.525267000000	-0.663696000000	-0.838652000000
C	-2.270305000000	-1.585313000000	1.025493000000
C	-3.313718000000	-1.661455000000	0.107810000000
H	-2.814239000000	1.199374000000	-1.620676000000
H	-0.615865000000	-0.404978000000	1.713695000000
H	-4.339794000000	-0.744110000000	-1.551592000000
H	-2.122311000000	-2.371471000000	1.759176000000
C	2.443503000000	3.484336000000	-0.089271000000
H	2.430310000000	4.530894000000	-0.392747000000
H	2.933896000000	3.398810000000	0.883503000000
C	-2.443596000000	3.484194000000	0.089146000000
H	-2.933892000000	3.398574000000	-0.883672000000
H	-2.998633000000	2.901002000000	0.827500000000
H	-2.430512000000	4.530769000000	0.392571000000
Cl	4.383738000000	-3.045022000000	-0.142718000000
Cl	-4.383708000000	-3.045062000000	0.142660000000
H	2.998517000000	2.901152000000	-0.827649000000

TS1 neutral singlet, imaginary frequency = 168.3*i* cm^{-1}

C	3.714775000000	-2.143559000000	-0.151458000000
O	3.585903000000	-2.963020000000	0.778053000000
C	4.674578000000	-0.985889000000	-0.042158000000
C	5.099992000000	-0.321086000000	-1.193524000000
C	5.148815000000	-0.580085000000	1.206252000000
C	5.971802000000	0.762910000000	-1.098807000000

H	4.730404000000	-0.644909000000	-2.165787000000
C	6.016137000000	0.507506000000	1.305608000000
C	6.424815000000	1.184428000000	0.153610000000
H	6.295720000000	1.281154000000	-1.997560000000
H	6.374830000000	0.829926000000	2.279592000000
H	7.099851000000	2.032499000000	0.230707000000
H	4.820514000000	-1.116106000000	2.093220000000
H	3.581393000000	-2.472365000000	-1.199555000000
N	1.470675000000	0.236317000000	-0.173163000000
C	1.897631000000	-1.043568000000	-0.276003000000
C	0.083140000000	0.305487000000	-0.090847000000
C	-0.365135000000	-0.985660000000	-0.128000000000
N	0.767514000000	-1.783899000000	-0.245203000000
C	-1.747824000000	-1.492436000000	-0.103497000000
C	-2.134296000000	-2.499172000000	0.789602000000
C	-2.704495000000	-0.947090000000	-0.969551000000
C	-3.447451000000	-2.961682000000	0.815741000000
C	-4.022658000000	-1.393660000000	-0.948072000000
C	-4.376541000000	-2.400268000000	-0.054981000000
H	-1.411737000000	-2.919146000000	1.483724000000
H	-2.415639000000	-0.170504000000	-1.673144000000
H	-3.743358000000	-3.741884000000	1.510001000000
H	-4.759419000000	-0.971051000000	-1.623917000000
C	-0.692068000000	1.553867000000	0.007227000000
C	-0.491356000000	2.596025000000	-0.906840000000
C	-1.674031000000	1.695286000000	0.995913000000
C	-1.246452000000	3.763279000000	-0.834073000000
C	-2.442755000000	2.853313000000	1.074709000000
C	-2.215562000000	3.875790000000	0.158226000000
H	0.252334000000	2.494885000000	-1.692904000000
H	-1.836164000000	0.896538000000	1.714864000000
H	-1.088142000000	4.567206000000	-1.546032000000
H	-3.201120000000	2.961274000000	1.843790000000
C	0.739220000000	-3.236509000000	-0.394940000000
H	-0.110515000000	-3.514161000000	-1.021607000000
H	1.661560000000	-3.556432000000	-0.875019000000
C	2.354178000000	1.399960000000	-0.128125000000
H	2.567353000000	1.760088000000	-1.137910000000
H	1.871125000000	2.192658000000	0.444799000000
H	3.283161000000	1.122030000000	0.367638000000
H	0.653191000000	-3.724348000000	0.577953000000
Cl	-3.168973000000	5.338613000000	0.260048000000
Cl	-6.029064000000	-2.974686000000	-0.026212000000

INT1 neutral singlet

C	-3.455415000000	-1.054942000000	-1.235760000000

O	-3.755919000000	-0.492548000000	-2.415090000000
C	-4.342317000000	-0.626974000000	-0.040791000000
C	-4.117015000000	-1.120536000000	1.249967000000
C	-5.403510000000	0.250482000000	-0.254222000000
C	-4.936707000000	-0.737651000000	2.310806000000
H	-3.291802000000	-1.811003000000	1.427479000000
C	-6.229467000000	0.637037000000	0.805176000000
C	-5.997886000000	0.145562000000	2.090181000000
H	-4.750823000000	-1.126554000000	3.308670000000
H	-7.054052000000	1.323037000000	0.627576000000
H	-6.638187000000	0.445668000000	2.915225000000
H	-5.561208000000	0.619876000000	-1.264131000000
H	-3.500418000000	-2.167620000000	-1.239331000000
N	-1.004443000000	-1.619771000000	-0.609857000000
C	-1.999454000000	-0.747661000000	-0.832915000000
C	0.178388000000	-0.926404000000	-0.380273000000
C	-0.128928000000	0.405496000000	-0.455999000000
N	-1.483809000000	0.485112000000	-0.737741000000
C	0.753635000000	1.573733000000	-0.303538000000
C	0.421579000000	2.616116000000	0.570099000000
C	1.960601000000	1.630468000000	-1.011184000000
C	1.276413000000	3.702582000000	0.734236000000
C	2.828050000000	2.706823000000	-0.849150000000
C	2.472005000000	3.731765000000	0.022584000000
H	-0.501532000000	2.577456000000	1.141556000000
H	2.223958000000	0.830084000000	-1.697349000000
H	1.018383000000	4.508803000000	1.413264000000
H	3.762874000000	2.749126000000	-1.398831000000
C	1.475796000000	-1.563230000000	-0.101466000000
C	1.992812000000	-2.548378000000	-0.951532000000
C	2.224796000000	-1.153024000000	1.008073000000
C	3.235326000000	-3.122660000000	-0.697422000000
C	3.472223000000	-1.712743000000	1.268259000000
C	3.960347000000	-2.694287000000	0.410708000000
H	1.430880000000	-2.862781000000	-1.827136000000
H	1.828986000000	-0.393479000000	1.676932000000
H	3.635985000000	-3.885094000000	-1.357780000000
H	4.050982000000	-1.394479000000	2.129408000000
C	-2.254660000000	1.711016000000	-0.947897000000
H	-3.082739000000	1.454709000000	-1.610770000000
H	-2.622276000000	2.089469000000	0.008968000000
C	-1.158088000000	-3.074783000000	-0.553624000000
H	-1.143117000000	-3.494375000000	-1.561731000000
H	-0.335677000000	-3.486002000000	0.030640000000
H	-2.096714000000	-3.319979000000	-0.058819000000
H	-1.608722000000	2.454590000000	-1.416948000000
Cl	3.554310000000	5.089407000000	0.230245000000

Cl	5.523876000000	-3.406777000000	0.733351000000

TS2 neutral singlet, imaginary frequency = 1202.7*i* cm^{-1}

C	-3.253521000000	0.001993000000	0.653713000000
C	-4.004904000000	-0.311333000000	-0.588680000000
C	-5.269507000000	-0.923029000000	-0.518230000000
C	-3.534856000000	0.075634000000	-1.859727000000
C	-6.029113000000	-1.136640000000	-1.668476000000
H	-5.647489000000	-1.234787000000	0.450549000000
C	-4.298461000000	-0.136472000000	-3.004971000000
C	-5.553820000000	-0.744186000000	-2.920595000000
H	-7.001944000000	-1.615165000000	-1.582453000000
H	-3.907934000000	0.173313000000	-3.971235000000
H	-6.146718000000	-0.912407000000	-3.815172000000
H	-2.558994000000	0.549258000000	-1.958843000000
H	-3.773225000000	1.266747000000	1.041871000000
O	-3.616049000000	-0.865192000000	1.730110000000
H	-3.679903000000	-0.315451000000	2.538954000000
O	-3.717322000000	1.050000000000	3.775385000000
O	-4.313114000000	2.235186000000	1.522160000000
H	-4.021138000000	1.648479000000	3.025505000000
H	-4.441209000000	1.017245000000	4.418053000000
H	-5.258162000000	2.150500000000	1.319839000000
N	-0.995159000000	1.057645000000	0.252090000000
C	-1.779230000000	-0.017437000000	0.454444000000
C	0.325945000000	0.659491000000	0.125180000000
C	0.339575000000	-0.704080000000	0.250660000000
N	-0.974346000000	-1.097917000000	0.441951000000
C	1.493338000000	-1.620531000000	0.237696000000
C	1.532971000000	-2.730519000000	-0.614351000000
C	2.589322000000	-1.354458000000	1.067495000000
C	2.643432000000	-3.570148000000	-0.631708000000
C	3.708487000000	-2.181601000000	1.054247000000
C	3.718330000000	-3.283779000000	0.204481000000
H	0.701987000000	-2.938661000000	-1.282414000000
H	2.568174000000	-0.495899000000	1.733361000000
H	2.672562000000	-4.430530000000	-1.292645000000
H	4.555600000000	-1.973095000000	1.700197000000
C	1.451892000000	1.579927000000	-0.107050000000
C	1.652985000000	2.694915000000	0.714830000000
C	2.360883000000	1.315019000000	-1.138711000000
C	2.740707000000	3.539252000000	0.510082000000
C	3.456739000000	2.146647000000	-1.348752000000
C	3.630728000000	3.250969000000	-0.520116000000
H	0.968569000000	2.900947000000	1.532885000000
H	2.209151000000	0.455300000000	-1.786195000000

H	2.897111000000	4.401937000000	1.150140000000
H	4.160114000000	1.941602000000	-2.149509000000
C	-1.439033000000	-2.481700000000	0.537120000000
H	-2.396670000000	-2.484899000000	1.052851000000
H	-1.545755000000	-2.901364000000	-0.465926000000
C	-1.472992000000	2.434302000000	0.119278000000
H	-1.366006000000	2.961775000000	1.069367000000
H	-0.885372000000	2.931154000000	-0.653951000000
H	-2.522274000000	2.420676000000	-0.167444000000
H	-0.710246000000	-3.061146000000	1.105945000000
Cl	5.004630000000	4.302493000000	-0.781433000000
Cl	5.114712000000	-4.334669000000	0.184939000000

BINT neutral singlet

C	-3.216490000000	-1.385286000000	-0.361261000000
O	-3.386025000000	-2.658971000000	-0.917530000000
C	-4.406228000000	-0.645357000000	0.004377000000
C	-4.384559000000	0.438338000000	0.915910000000
C	-5.670701000000	-1.049724000000	-0.483493000000
C	-5.551700000000	1.102066000000	1.275414000000
H	-3.442887000000	0.740740000000	1.367686000000
C	-6.835971000000	-0.383409000000	-0.111377000000
C	-6.791562000000	0.703866000000	0.763720000000
H	-5.495529000000	1.929109000000	1.979230000000
H	-7.789394000000	-0.717362000000	-0.513865000000
H	-7.701317000000	1.222649000000	1.051200000000
H	-5.728251000000	-1.886087000000	-1.174006000000
H	-3.822958000000	-3.239735000000	-0.270542000000
N	-1.442237000000	0.354266000000	-0.306512000000
C	-1.907456000000	-0.947528000000	-0.261966000000
C	-0.044185000000	0.339855000000	-0.186186000000
C	0.350313000000	-0.958183000000	-0.088845000000
N	-0.795697000000	-1.758780000000	-0.145963000000
C	1.699786000000	-1.520245000000	0.052343000000
C	2.099282000000	-2.608115000000	-0.736383000000
C	2.610922000000	-0.971354000000	0.964274000000
C	3.384916000000	-3.130862000000	-0.630984000000
C	3.902125000000	-1.479207000000	1.073417000000
C	4.274060000000	-2.554501000000	0.271744000000
H	1.404500000000	-3.045610000000	-1.449002000000
H	2.308815000000	-0.143129000000	1.599351000000
H	3.690768000000	-3.970155000000	-1.247545000000
H	4.604943000000	-1.050371000000	1.780677000000
C	0.750441000000	1.573435000000	-0.190784000000
C	0.330767000000	2.684296000000	0.555197000000
C	1.938928000000	1.662390000000	-0.928643000000

C	1.085170000000	3.853536000000	0.579913000000
C	2.707500000000	2.822334000000	-0.904334000000
C	2.270463000000	3.906090000000	-0.147921000000
H	-0.587551000000	2.632764000000	1.134660000000
H	2.265387000000	0.821075000000	-1.533667000000
H	0.757901000000	4.708328000000	1.163342000000
H	3.627576000000	2.884829000000	-1.476841000000
C	-0.877507000000	-3.114435000000	0.378651000000
H	-1.688575000000	-3.163415000000	1.112160000000
H	-1.067375000000	-3.840218000000	-0.414447000000
C	-2.166155000000	1.430784000000	-0.966104000000
H	-2.656255000000	2.098240000000	-0.251468000000
H	-1.468662000000	2.008992000000	-1.575496000000
H	-2.927659000000	0.990065000000	-1.614995000000
H	0.060787000000	-3.358263000000	0.878269000000
Cl	3.229065000000	5.369624000000	-0.117034000000
Cl	5.894259000000	-3.200905000000	0.407787000000

TS3 neutral singlet, imaginary frequency = 191.1*i* cm^{-1}

C	1.087146000000	0.552629000000	-0.534776000000
C	1.285937000000	-0.795117000000	-0.510899000000
C	-0.881212000000	-0.436952000000	-0.992675000000
N	0.065055000000	-1.394044000000	-0.797641000000
N	-0.247967000000	0.763389000000	-0.869632000000
C	-2.288351000000	-0.689664000000	-1.234250000000
O	-2.503633000000	-1.627866000000	-2.223177000000
H	-2.962772000000	-2.393923000000	-1.760011000000
C	-2.914151000000	-2.097263000000	0.436502000000
O	-3.309024000000	-3.040394000000	-0.314152000000
H	-1.899307000000	-2.130834000000	0.869924000000
C	-3.872468000000	-1.319798000000	1.258361000000
C	-5.231872000000	-1.271132000000	0.923469000000
C	-3.418455000000	-0.630066000000	2.386241000000
C	-6.118428000000	-0.526766000000	1.697360000000
C	-4.307324000000	0.103138000000	3.172159000000
C	-5.657817000000	0.162199000000	2.824329000000
H	-5.579242000000	-1.817277000000	0.050172000000
H	-2.360800000000	-0.665964000000	2.643839000000
H	-7.170365000000	-0.483422000000	1.426942000000
H	-3.947733000000	0.632082000000	4.050864000000
H	-6.350870000000	0.739917000000	3.430061000000
C	-3.292385000000	0.378766000000	-1.128452000000
C	-4.408317000000	0.380467000000	-1.982973000000
C	-3.261609000000	1.341057000000	-0.096915000000
C	-5.434582000000	1.315319000000	-1.827908000000
C	-4.279208000000	2.273721000000	0.051589000000

C	-5.379650000000	2.270094000000	-0.814103000000
H	-4.466883000000	-0.362105000000	-2.772851000000
H	-2.437958000000	1.342392000000	0.613556000000
H	-6.283259000000	1.292034000000	-2.507475000000
H	-4.225074000000	2.999106000000	0.860286000000
H	-6.178586000000	2.996182000000	-0.692543000000
C	-0.107327000000	-2.843388000000	-0.896255000000
H	-1.156941000000	-3.107878000000	-0.813166000000
H	0.267819000000	-3.192716000000	-1.861271000000
H	0.454042000000	-3.317564000000	-0.089182000000
C	-0.704782000000	2.034040000000	-1.439961000000
H	-1.105921000000	2.700813000000	-0.675518000000
H	0.150842000000	2.506816000000	-1.924553000000
H	-1.469684000000	1.834223000000	-2.188363000000
C	2.037248000000	1.646088000000	-0.288785000000
C	1.676101000000	2.733435000000	0.517431000000
C	3.321463000000	1.605157000000	-0.846350000000
C	2.578325000000	3.763201000000	0.766662000000
C	4.235870000000	2.624268000000	-0.597062000000
C	3.850702000000	3.693185000000	0.206837000000
H	0.686689000000	2.774007000000	0.965377000000
H	3.608671000000	0.775945000000	-1.487195000000
H	2.296100000000	4.603795000000	1.392617000000
H	5.230322000000	2.590216000000	-1.030794000000
C	2.516494000000	-1.539219000000	-0.187966000000
C	3.183705000000	-1.277870000000	1.014697000000
C	3.057550000000	-2.469934000000	-1.083115000000
C	4.372722000000	-1.932467000000	1.323993000000
C	4.241125000000	-3.137656000000	-0.782140000000
C	4.884471000000	-2.858627000000	0.420125000000
H	2.770890000000	-0.558321000000	1.716790000000
H	2.565572000000	-2.664798000000	-2.031759000000
H	4.887464000000	-1.729076000000	2.257779000000
H	4.660027000000	-3.856558000000	-1.479084000000
Cl	6.373024000000	-3.692094000000	0.805134000000
Cl	4.990098000000	4.983182000000	0.516871000000

INT2 neutral singlet

C	2.480193000000	-0.791922000000	-0.240509000000
O	2.699281000000	-2.044224000000	-0.682356000000
C	2.990942000000	-0.589177000000	1.204570000000
C	3.689605000000	0.528128000000	1.672135000000
C	2.724331000000	-1.629349000000	2.105694000000
C	4.112777000000	0.603025000000	3.002831000000
H	3.926007000000	1.352247000000	1.005821000000
C	3.135454000000	-1.556043000000	3.434259000000

C	3.836915000000	-0.436127000000	3.888683000000
H	4.662844000000	1.477276000000	3.340671000000
H	2.915250000000	-2.374168000000	4.115001000000
H	4.166920000000	-0.377475000000	4.922149000000
H	2.198666000000	-2.508843000000	1.741796000000
C	7.395432000000	0.593191000000	-1.280769000000
C	6.576192000000	1.720318000000	-1.337316000000
C	5.187788000000	1.572196000000	-1.341447000000
C	4.597022000000	0.305825000000	-1.287370000000
C	5.428406000000	-0.821592000000	-1.241608000000
C	6.815542000000	-0.677142000000	-1.233854000000
H	8.476567000000	0.701970000000	-1.276026000000
H	7.014923000000	2.713781000000	-1.378342000000
H	4.552128000000	2.455594000000	-1.377523000000
H	4.970371000000	-1.805200000000	-1.196219000000
H	7.448519000000	-1.559847000000	-1.191128000000
C	3.082275000000	0.191145000000	-1.329150000000
O	2.660396000000	-0.361617000000	-2.565532000000
H	2.673911000000	1.201825000000	-1.271496000000
H	2.637404000000	-1.325814000000	-2.331533000000
N	0.312933000000	0.700515000000	-0.049822000000
C	0.926855000000	-0.497212000000	-0.177523000000
C	-1.063129000000	0.529408000000	-0.056550000000
C	-1.289447000000	-0.810018000000	-0.166132000000
N	-0.048376000000	-1.425535000000	-0.240780000000
C	-2.581096000000	-1.517880000000	-0.241678000000
C	-2.926836000000	-2.498755000000	0.695146000000
C	-3.499443000000	-1.165271000000	-1.237066000000
C	-4.167255000000	-3.127712000000	0.636198000000
C	-4.746247000000	-1.781837000000	-1.303466000000
C	-5.062003000000	-2.758795000000	-0.364542000000
H	-2.232742000000	-2.765853000000	1.486857000000
H	-3.238521000000	-0.403773000000	-1.967134000000
H	-4.435357000000	-3.886886000000	1.363957000000
H	-5.456944000000	-1.508507000000	-2.076777000000
C	-2.041895000000	1.625228000000	0.042497000000
C	-1.991472000000	2.718702000000	-0.830624000000
C	-3.065344000000	1.553456000000	0.994779000000
C	-2.943669000000	3.730925000000	-0.752458000000
C	-4.027639000000	2.556005000000	1.078886000000
C	-3.951674000000	3.634445000000	0.202724000000
H	-1.213560000000	2.777589000000	-1.587318000000
H	-3.108539000000	0.710907000000	1.679793000000
H	-2.905880000000	4.577210000000	-1.430785000000
H	-4.819333000000	2.500325000000	1.819328000000
C	0.072989000000	-2.886409000000	-0.360436000000
H	-0.678759000000	-3.229639000000	-1.072969000000

H	1.081210000000	-3.107693000000	-0.696258000000
C	0.927024000000	2.006099000000	0.205525000000
H	1.050460000000	2.562876000000	-0.724993000000
H	0.270732000000	2.559068000000	0.878165000000
H	1.886912000000	1.871822000000	0.694550000000
H	-0.112970000000	-3.340213000000	0.615492000000
Cl	-5.152457000000	4.900927000000	0.302760000000
Cl	-6.623724000000	-3.541152000000	-0.441368000000

TS4 neutral singlet, imaginary frequency = 124.6*i* cm^{-1}

C	2.910403000000	-0.800569000000	0.313247000000
O	2.905311000000	-1.908907000000	0.895285000000
C	2.900320000000	0.451801000000	1.162921000000
C	3.588767000000	1.615666000000	0.813851000000
C	2.184977000000	0.420319000000	2.366119000000
C	3.566019000000	2.730205000000	1.656258000000
H	4.142374000000	1.672805000000	-0.118274000000
C	2.145569000000	1.534938000000	3.198048000000
C	2.842414000000	2.695498000000	2.846053000000
H	4.112492000000	3.626346000000	1.375417000000
H	1.575093000000	1.501374000000	4.122330000000
H	2.819548000000	3.564982000000	3.497166000000
H	1.648795000000	-0.486586000000	2.634964000000
C	7.918803000000	-0.346742000000	-0.716618000000
C	7.196213000000	0.449578000000	-1.604950000000
C	5.810378000000	0.311276000000	-1.695690000000
C	5.129634000000	-0.618609000000	-0.904732000000
C	5.863634000000	-1.419000000000	-0.021057000000
C	7.248040000000	-1.282272000000	0.073443000000
H	8.997515000000	-0.240418000000	-0.640491000000
H	7.709111000000	1.178937000000	-2.226285000000
H	5.247703000000	0.937821000000	-2.385740000000
H	5.347909000000	-2.149136000000	0.597378000000
H	7.805702000000	-1.906649000000	0.766561000000
C	3.620789000000	-0.776755000000	-1.057381000000
O	3.325180000000	-1.996557000000	-1.712839000000
H	3.240514000000	0.041510000000	-1.675640000000
H	3.170404000000	-2.634733000000	-0.988702000000
N	0.190619000000	0.625204000000	-0.526587000000
C	0.882238000000	-0.533038000000	-0.409428000000
C	-1.177981000000	0.422860000000	-0.401112000000
C	-1.346443000000	-0.920349000000	-0.210991000000
N	-0.070629000000	-1.474291000000	-0.217445000000
C	-2.595123000000	-1.671843000000	0.003929000000
C	-3.501874000000	-1.232733000000	0.977144000000
C	-2.917513000000	-2.794598000000	-0.768855000000

C	-4.710377000000	-1.893392000000	1.177130000000
C	-4.118911000000	-3.471069000000	-0.573001000000
C	-5.002272000000	-3.008822000000	0.398080000000
H	-3.259540000000	-0.366967000000	1.587806000000
H	-2.235764000000	-3.139410000000	-1.541473000000
H	-5.409723000000	-1.547076000000	1.931600000000
H	-4.366780000000	-4.339294000000	-1.175493000000
C	-2.198655000000	1.479153000000	-0.506766000000
C	-3.292285000000	1.299497000000	-1.363282000000
C	-2.121433000000	2.647108000000	0.262476000000
C	-4.297680000000	2.258314000000	-1.448500000000
C	-3.115318000000	3.618929000000	0.180224000000
C	-4.194030000000	3.409319000000	-0.673445000000
H	-3.358036000000	0.402208000000	-1.972918000000
H	-1.291046000000	2.795729000000	0.947873000000
H	-5.143435000000	2.113479000000	-2.113524000000
H	-3.055866000000	4.520902000000	0.781066000000
C	0.206237000000	-2.899006000000	-0.058107000000
H	1.214634000000	-3.007607000000	0.336515000000
H	-0.508650000000	-3.330123000000	0.645244000000
C	0.804754000000	1.915241000000	-0.814176000000
H	1.772013000000	1.739950000000	-1.283863000000
H	0.167733000000	2.472215000000	-1.504501000000
H	0.944329000000	2.493224000000	0.103669000000
H	0.121441000000	-3.410601000000	-1.020447000000
Cl	-5.451329000000	4.622149000000	-0.768582000000
Cl	-6.517383000000	-3.849267000000	0.642901000000

4,5-bis(p-aminophenyl)-1,3-dimethylimdazolylidene

Carbene neutral singlet

N	-1.062983000000	2.673804000000	0.027192000000
C	0.000082000000	3.519861000000	-0.000041000000
C	-0.683737000000	1.333561000000	0.015850000000
C	0.683802000000	1.333543000000	-0.015998000000
N	1.063110000000	2.673754000000	-0.027215000000
C	1.616000000000	0.194870000000	-0.066132000000
C	2.667599000000	0.063801000000	0.851687000000
C	1.448715000000	-0.816237000000	-1.023561000000
C	3.524883000000	-1.030084000000	0.813583000000
C	2.295180000000	-1.917826000000	-1.064195000000
C	3.351171000000	-2.040369000000	-0.146274000000
H	2.811397000000	0.819673000000	1.619754000000
H	0.643698000000	-0.735614000000	-1.750433000000
H	4.333004000000	-1.114503000000	1.536234000000

H	2.149193000000	-2.690781000000	-1.815143000000
C	-1.615953000000	0.194902000000	0.066088000000
C	-2.667536000000	0.063777000000	-0.851808000000
C	-1.448766000000	-0.816158000000	1.023532000000
C	-3.524918000000	-1.029968000000	-0.813604000000
C	-2.295271000000	-1.917735000000	1.064221000000
C	-3.351326000000	-2.040276000000	0.146355000000
H	-2.811169000000	0.819565000000	-1.619988000000
H	-0.643773000000	-0.735595000000	1.750444000000
H	-4.333099000000	-1.114397000000	-1.536192000000
H	-2.149184000000	-2.690696000000	1.815139000000
C	2.442606000000	3.133834000000	-0.094834000000
H	2.432173000000	4.187651000000	-0.373105000000
H	2.942113000000	3.022920000000	0.870961000000
C	-2.442446000000	3.133964000000	0.094979000000
H	-2.941969000000	3.023464000000	-0.870855000000
H	-2.990155000000	2.565547000000	0.850511000000
H	-2.431937000000	4.187676000000	0.373647000000
H	2.990274000000	2.565656000000	-0.850579000000
N	4.165668000000	-3.168647000000	-0.147019000000
H	4.224895000000	-3.650137000000	-1.038712000000
H	5.084008000000	-3.032627000000	0.263236000000
N	-4.165901000000	-3.168278000000	0.147272000000
H	-4.225551000000	-3.650048000000	1.038732000000
H	-5.083692000000	-3.032941000000	-0.264346000000

TS1 neutral singlet, imaginary frequency = 191.9*i* cm^{-1}

C	3.213420000000	-2.057768000000	0.361833000000
O	2.882178000000	-2.440944000000	1.500677000000
C	4.229553000000	-0.961666000000	0.173008000000
C	4.876632000000	-0.819123000000	-1.056320000000
C	4.541894000000	-0.097971000000	1.222977000000
C	5.809743000000	0.198723000000	-1.246846000000
H	4.632302000000	-1.498899000000	-1.871564000000
C	5.471559000000	0.924703000000	1.034892000000
C	6.103370000000	1.078052000000	-0.201326000000
H	6.306945000000	0.308773000000	-2.206898000000
H	5.704879000000	1.603057000000	1.851463000000
H	6.828166000000	1.874202000000	-0.347638000000
H	4.040243000000	-0.227427000000	2.178785000000
H	3.204680000000	-2.768358000000	-0.484658000000
N	1.112519000000	0.242078000000	-0.338446000000
C	1.492036000000	-1.055872000000	-0.390498000000
C	-0.269560000000	0.368223000000	-0.195307000000
C	-0.764354000000	-0.907388000000	-0.165846000000
N	0.337466000000	-1.749984000000	-0.282068000000

C	-2.155266000000	-1.370613000000	-0.035316000000
C	-2.970074000000	-0.898233000000	1.002393000000
C	-2.712399000000	-2.267413000000	-0.957463000000
C	-4.294207000000	-1.303958000000	1.117621000000
C	-4.033421000000	-2.684184000000	-0.846169000000
C	-4.846662000000	-2.208056000000	0.195103000000
H	-2.558748000000	-0.205919000000	1.733429000000
H	-2.107275000000	-2.638318000000	-1.781693000000
H	-4.911079000000	-0.929006000000	1.930929000000
H	-4.448519000000	-3.379976000000	-1.571483000000
C	-0.990616000000	1.650229000000	-0.144401000000
C	-2.101858000000	1.869851000000	-0.970900000000
C	-0.615579000000	2.670950000000	0.740321000000
C	-2.814943000000	3.061183000000	-0.917299000000
C	-1.316962000000	3.869768000000	0.794264000000
C	-2.430641000000	4.083819000000	-0.034241000000
H	-2.410487000000	1.095596000000	-1.669624000000
H	0.230837000000	2.523616000000	1.406841000000
H	-3.673497000000	3.212270000000	-1.567537000000
H	-1.010437000000	4.649354000000	1.487698000000
C	0.278068000000	-3.206716000000	-0.250779000000
H	0.151801000000	-3.609718000000	-1.258890000000
H	1.201444000000	-3.581048000000	0.190397000000
C	2.022526000000	1.373848000000	-0.484050000000
H	1.536514000000	2.149775000000	-1.079220000000
H	2.293597000000	1.784226000000	0.491863000000
H	2.921329000000	1.036682000000	-0.999438000000
H	-0.563165000000	-3.519187000000	0.370322000000
N	-3.174771000000	5.254835000000	0.064104000000
H	-2.665952000000	6.056886000000	0.421711000000
H	-3.712185000000	5.491598000000	-0.763560000000
N	-6.186180000000	-2.574933000000	0.274218000000
H	-6.411461000000	-3.461073000000	-0.166317000000
H	-6.594132000000	-2.505856000000	1.201106000000

INT1 neutral singlet

C	-3.049181000000	-1.021215000000	-1.247575000000
O	-3.329610000000	-0.486434000000	-2.445443000000
C	-3.968391000000	-0.575941000000	-0.083310000000
C	-3.761909000000	-1.026462000000	1.226265000000
C	-5.041822000000	0.273431000000	-0.344529000000
C	-4.611593000000	-0.628925000000	2.257791000000
H	-2.926654000000	-1.693523000000	1.442146000000
C	-5.898057000000	0.674379000000	0.685093000000
C	-5.685044000000	0.225669000000	1.988790000000
H	-4.439311000000	-0.983932000000	3.270628000000

H	-6.731757000000	1.338209000000	0.469580000000
H	-6.348580000000	0.537191000000	2.790925000000
H	-5.183560000000	0.610773000000	-1.367911000000
H	-3.089179000000	-2.134352000000	-1.228588000000
N	-0.610796000000	-1.562498000000	-0.565012000000
C	-1.605732000000	-0.699168000000	-0.817573000000
C	0.565791000000	-0.860255000000	-0.312536000000
C	0.252153000000	0.470212000000	-0.407496000000
N	-1.099547000000	0.536834000000	-0.720731000000
C	1.118921000000	1.647853000000	-0.252975000000
C	0.769914000000	2.704408000000	0.599308000000
C	2.341468000000	1.720112000000	-0.935250000000
C	1.608784000000	3.799809000000	0.762304000000
C	3.189707000000	2.807659000000	-0.771835000000
C	2.835130000000	3.868194000000	0.079568000000
H	-0.164876000000	2.666901000000	1.153377000000
H	2.629018000000	0.914310000000	-1.606519000000
H	1.323035000000	4.610208000000	1.428321000000
H	4.133534000000	2.848720000000	-1.309981000000
C	1.855823000000	-1.491646000000	0.002960000000
C	2.414583000000	-2.469001000000	-0.832187000000
C	2.578509000000	-1.093220000000	1.135976000000
C	3.649018000000	-3.036998000000	-0.543417000000
C	3.817455000000	-1.649373000000	1.427581000000
C	4.372010000000	-2.634391000000	0.592356000000
H	1.880745000000	-2.784604000000	-1.725949000000
H	2.161214000000	-0.339573000000	1.799720000000
H	4.067857000000	-3.794579000000	-1.201182000000
H	4.364338000000	-1.330474000000	2.311600000000
C	-1.872258000000	1.754379000000	-0.960848000000
H	-2.685583000000	1.487800000000	-1.637786000000
H	-2.262118000000	2.144152000000	-0.017189000000
C	-0.757722000000	-3.016769000000	-0.503814000000
H	-0.757396000000	-3.440013000000	-1.510716000000
H	0.078238000000	-3.421791000000	0.065176000000
H	-1.686441000000	-3.267804000000	0.007464000000
H	-1.220075000000	2.496370000000	-1.423981000000
N	3.705589000000	4.929721000000	0.290073000000
H	4.369349000000	5.097944000000	-0.459062000000
H	3.268280000000	5.788971000000	0.607068000000
N	5.634027000000	-3.153521000000	0.849204000000
H	5.932142000000	-3.102565000000	1.818005000000
H	5.814416000000	-4.067063000000	0.445775000000

TS2 neutral singlet, imaginary frequency = 1032.4*i* cm^{-1}

C	-2.865741000000	-0.370295000000	-0.586302000000
C	-3.599402000000	0.403957000000	0.443389000000
C	-4.846653000000	0.987042000000	0.156817000000
C	-3.119746000000	0.502887000000	1.765754000000
C	-5.577621000000	1.643722000000	1.147813000000
H	-5.232829000000	0.924133000000	-0.856136000000
C	-3.852691000000	1.157680000000	2.751779000000
C	-5.089720000000	1.735771000000	2.452288000000
H	-6.537197000000	2.089569000000	0.895658000000
H	-3.453622000000	1.220729000000	3.761323000000
H	-5.659061000000	2.249315000000	3.221777000000
H	-2.159025000000	0.058480000000	2.025566000000
H	-3.441271000000	-1.695664000000	-0.432231000000
O	-3.218918000000	0.043143000000	-1.913648000000
H	-3.342378000000	-0.768530000000	-2.446814000000
O	-3.539428000000	-2.513660000000	-3.039026000000
O	-4.021981000000	-2.726736000000	-0.459602000000
H	-3.813472000000	-2.764424000000	-2.107682000000
H	-4.307657000000	-2.673629000000	-3.606955000000
H	-4.942968000000	-2.522913000000	-0.232765000000
N	-0.528039000000	-1.233707000000	-0.099334000000
C	-1.391189000000	-0.254101000000	-0.416902000000
C	0.761615000000	-0.726461000000	-0.034441000000
C	0.671276000000	0.613418000000	-0.321718000000
N	-0.669821000000	0.875158000000	-0.548458000000
C	1.743122000000	1.614870000000	-0.429169000000
C	1.673645000000	2.845275000000	0.238435000000
C	2.892620000000	1.330670000000	-1.180482000000
C	2.710004000000	3.766557000000	0.150910000000
C	3.936097000000	2.242440000000	-1.266831000000
C	3.859853000000	3.478978000000	-0.603454000000
H	0.806060000000	3.084331000000	0.848721000000
H	2.969491000000	0.380790000000	-1.704721000000
H	2.639954000000	4.716240000000	0.675675000000
H	4.818719000000	2.006456000000	-1.856288000000
C	1.948804000000	-1.523126000000	0.310638000000
C	2.264081000000	-2.704445000000	-0.373959000000
C	2.819807000000	-1.084483000000	1.317290000000
C	3.408146000000	-3.428528000000	-0.061756000000
C	3.968749000000	-1.798533000000	1.631301000000
C	4.280584000000	-2.985180000000	0.946453000000
H	1.612018000000	-3.059486000000	-1.168789000000
H	2.590942000000	-0.172957000000	1.864710000000
H	3.640048000000	-4.342101000000	-0.603937000000
H	4.632995000000	-1.445468000000	2.416381000000

C	-1.248915000000	2.171224000000	-0.891602000000
H	-2.172701000000	1.997706000000	-1.441800000000
H	-1.452249000000	2.743787000000	0.016801000000
C	-0.903053000000	-2.620249000000	0.171414000000
H	-0.202892000000	-3.032324000000	0.898464000000
H	-1.914144000000	-2.644870000000	0.573154000000
H	-0.864430000000	-3.204228000000	-0.751294000000
H	-0.543419000000	2.716173000000	-1.520692000000
N	5.457237000000	-3.670335000000	1.217365000000
H	5.842543000000	-3.519441000000	2.143926000000
H	5.452879000000	-4.653276000000	0.964932000000
N	4.870273000000	4.420531000000	-0.742604000000
H	4.923080000000	5.110435000000	-0.000295000000
H	5.783640000000	4.043117000000	-0.973256000000

BINT neutral singlet

C	-2.853705000000	-1.277762000000	-0.379106000000
O	-3.022099000000	-2.545650000000	-0.952947000000
C	-4.040051000000	-0.541421000000	-0.011628000000
C	-4.019938000000	0.551166000000	0.892486000000
C	-5.308967000000	-0.952988000000	-0.487635000000
C	-5.187533000000	1.212437000000	1.253497000000
H	-3.077852000000	0.860877000000	1.338144000000
C	-6.473917000000	-0.287579000000	-0.113913000000
C	-6.430043000000	0.807029000000	0.752561000000
H	-5.129757000000	2.044716000000	1.951219000000
H	-7.428235000000	-0.628691000000	-0.508666000000
H	-7.339954000000	1.324823000000	1.041225000000
H	-5.368638000000	-1.794758000000	-1.171309000000
H	-3.447022000000	-3.139164000000	-0.309648000000
N	-1.065301000000	0.449052000000	-0.312570000000
C	-1.538358000000	-0.845905000000	-0.264602000000
C	0.334760000000	0.430058000000	-0.176500000000
C	0.719424000000	-0.869517000000	-0.062794000000
N	-0.437110000000	-1.661403000000	-0.127733000000
C	2.060997000000	-1.443045000000	0.105439000000
C	2.478787000000	-2.536309000000	-0.667627000000
C	2.967689000000	-0.902944000000	1.028318000000
C	3.756994000000	-3.065083000000	-0.534099000000
C	4.250602000000	-1.419865000000	1.161948000000
C	4.667019000000	-2.510836000000	0.381284000000
H	1.795055000000	-2.976303000000	-1.390684000000
H	2.662326000000	-0.067475000000	1.653722000000
H	4.063664000000	-3.911461000000	-1.144087000000
H	4.939812000000	-0.986927000000	1.883070000000
C	1.134158000000	1.660970000000	-0.193712000000

C	0.733728000000	2.785204000000	0.543690000000
C	2.320677000000	1.748795000000	-0.936042000000
C	1.492389000000	3.949604000000	0.550313000000
C	3.090295000000	2.905823000000	-0.926825000000
C	2.687843000000	4.027290000000	-0.182899000000
H	-0.182743000000	2.745918000000	1.128742000000
H	2.643371000000	0.899980000000	-1.534105000000
H	1.165573000000	4.809264000000	1.130541000000
H	4.007290000000	2.954266000000	-1.509329000000
C	-0.534382000000	-3.018219000000	0.387304000000
H	-1.359361000000	-3.068678000000	1.105276000000
H	-0.711846000000	-3.740624000000	-0.412176000000
C	-1.779607000000	1.531002000000	-0.970666000000
H	-2.260734000000	2.205671000000	-0.256440000000
H	-1.076635000000	2.100951000000	-1.581565000000
H	-2.548185000000	1.097796000000	-1.616345000000
H	0.394338000000	-3.267197000000	0.902107000000
N	3.484776000000	5.167492000000	-0.127079000000
H	4.098443000000	5.295806000000	-0.925480000000
H	2.987538000000	6.022971000000	0.099476000000
N	5.969214000000	-2.993749000000	0.470355000000
H	6.430495000000	-2.814395000000	1.356572000000
H	6.085628000000	-3.959356000000	0.179745000000

TS3 neutral singlet, imaginary frequency = 159.9*i* cm^{-1}

C	1.458444000000	0.604818000000	-0.461186000000
C	1.665544000000	-0.742165000000	-0.426614000000
C	-0.494001000000	-0.400850000000	-0.972246000000
N	0.453103000000	-1.349924000000	-0.747647000000
N	0.128343000000	0.804344000000	-0.834710000000
C	-1.889372000000	-0.658211000000	-1.255427000000
O	-2.082715000000	-1.616407000000	-2.230834000000
H	-2.551000000000	-2.375070000000	-1.772662000000
C	-2.564069000000	-2.093241000000	0.450090000000
O	-2.937118000000	-3.028471000000	-0.313497000000
H	-1.550872000000	-2.108924000000	0.887734000000
C	-3.535353000000	-1.301209000000	1.237735000000
C	-4.889237000000	-1.262061000000	0.879049000000
C	-3.100068000000	-0.586929000000	2.358285000000
C	-5.789254000000	-0.504513000000	1.623848000000
C	-4.003254000000	0.158228000000	3.115814000000
C	-5.348296000000	0.206281000000	2.745168000000
H	-5.220982000000	-1.826200000000	0.011246000000
H	-2.046337000000	-0.614717000000	2.632280000000
H	-6.836664000000	-0.467982000000	1.335498000000
H	-3.659537000000	0.705875000000	3.989306000000

H	-6.052669000000	0.793097000000	3.328718000000
C	-2.909687000000	0.388888000000	-1.164610000000
C	-4.023071000000	0.363715000000	-2.024893000000
C	-2.902447000000	1.365001000000	-0.143809000000
C	-5.063820000000	1.284791000000	-1.887627000000
C	-3.934966000000	2.283460000000	-0.014029000000
C	-5.030210000000	2.254016000000	-0.886437000000
H	-4.065928000000	-0.388614000000	-2.806657000000
H	-2.083945000000	1.386243000000	0.572255000000
H	-5.907427000000	1.239749000000	-2.572628000000
H	-3.896968000000	3.018686000000	0.786923000000
H	-5.840178000000	2.970100000000	-0.779279000000
C	0.292558000000	-2.798932000000	-0.844494000000
H	-0.756453000000	-3.071095000000	-0.780461000000
H	0.688710000000	-3.151727000000	-1.800132000000
H	0.843102000000	-3.266476000000	-0.026136000000
C	-0.319071000000	2.064143000000	-1.431353000000
H	-0.739347000000	2.741883000000	-0.686734000000
H	0.545990000000	2.534145000000	-1.902093000000
H	-1.067806000000	1.852058000000	-2.193128000000
C	2.389540000000	1.708943000000	-0.197904000000
C	2.007613000000	2.804078000000	0.590474000000
C	3.692530000000	1.686870000000	-0.715226000000
C	2.893138000000	3.841326000000	0.854434000000
C	4.586940000000	2.715263000000	-0.448003000000
C	4.200639000000	3.812108000000	0.341108000000
H	1.005284000000	2.843062000000	1.011428000000
H	4.007224000000	0.855947000000	-1.342205000000
H	2.580192000000	4.682336000000	1.468563000000
H	5.593553000000	2.681746000000	-0.857923000000
C	2.885945000000	-1.483652000000	-0.067769000000
C	3.529876000000	-1.229420000000	1.150711000000
C	3.464768000000	-2.412403000000	-0.943433000000
C	4.710332000000	-1.880382000000	1.487235000000
C	4.640281000000	-3.074040000000	-0.611527000000
C	5.283157000000	-2.817613000000	0.611341000000
H	3.100904000000	-0.509201000000	1.843679000000
H	3.000046000000	-2.609289000000	-1.906472000000
H	5.196224000000	-1.672793000000	2.437692000000
H	5.075391000000	-3.790813000000	-1.303739000000
N	6.425491000000	-3.520498000000	0.973687000000
H	7.015914000000	-3.057010000000	1.656833000000
H	6.967077000000	-3.889086000000	0.198519000000
N	5.109345000000	4.815166000000	0.656222000000
H	4.695436000000	5.709056000000	0.900347000000
H	5.874972000000	4.922583000000	-0.001218000000

INT2 neutral singlet

C	2.098939000000	-0.769546000000	-0.252719000000
O	2.315127000000	-2.019841000000	-0.705415000000
C	2.604847000000	-0.588878000000	1.197448000000
C	3.321978000000	0.509249000000	1.681997000000
C	2.314098000000	-1.633706000000	2.086002000000
C	3.740234000000	0.560680000000	3.015526000000
H	3.575545000000	1.337573000000	1.027349000000
C	2.719654000000	-1.583678000000	3.417223000000
C	3.440591000000	-0.482898000000	3.888119000000
H	4.304666000000	1.420730000000	3.366014000000
H	2.479877000000	-2.405047000000	4.087395000000
H	3.766555000000	-0.442393000000	4.923731000000
H	1.773215000000	-2.498682000000	1.709707000000
C	7.028786000000	0.610391000000	-1.241256000000
C	6.213271000000	1.740118000000	-1.300158000000
C	4.824493000000	1.596016000000	-1.317589000000
C	4.229670000000	0.331097000000	-1.274557000000
C	5.057439000000	-0.798914000000	-1.226456000000
C	6.444846000000	-0.658536000000	-1.205525000000
H	8.110144000000	0.716028000000	-1.226101000000
H	6.655233000000	2.732485000000	-1.332595000000
H	4.191603000000	2.481367000000	-1.355125000000
H	4.595725000000	-1.781243000000	-1.189531000000
H	7.074983000000	-1.543203000000	-1.161006000000
C	2.715136000000	0.219985000000	-1.328782000000
O	2.303875000000	-0.324432000000	-2.572507000000
H	2.307621000000	1.230929000000	-1.267923000000
H	2.270967000000	-1.289475000000	-2.340442000000
N	-0.050826000000	0.738217000000	-0.044896000000
C	0.550017000000	-0.463097000000	-0.196374000000
C	-1.431732000000	0.585323000000	-0.058348000000
C	-1.673431000000	-0.749896000000	-0.200954000000
N	-0.435539000000	-1.377450000000	-0.283990000000
C	-2.968414000000	-1.443888000000	-0.305417000000
C	-3.344423000000	-2.444376000000	0.600860000000
C	-3.882118000000	-1.069002000000	-1.299225000000
C	-4.587440000000	-3.058609000000	0.513091000000
C	-5.129899000000	-1.673184000000	-1.390863000000
C	-5.501724000000	-2.681626000000	-0.485910000000
H	-2.661350000000	-2.740595000000	1.393078000000
H	-3.609567000000	-0.293582000000	-2.011395000000
H	-4.864685000000	-3.832322000000	1.224910000000
H	-5.826678000000	-1.371233000000	-2.168903000000
C	-2.392346000000	1.690617000000	0.078289000000
C	-2.341229000000	2.816402000000	-0.755366000000

C	-3.418083000000	1.613744000000	1.030375000000
C	-3.277314000000	3.835998000000	-0.638406000000
C	-4.361908000000	2.625713000000	1.150079000000
C	-4.305025000000	3.756316000000	0.317289000000
H	-1.564667000000	2.893890000000	-1.512850000000
H	-3.473043000000	0.750809000000	1.689916000000
H	-3.225239000000	4.701961000000	-1.293758000000
H	-5.150188000000	2.551267000000	1.895186000000
C	-0.329819000000	-2.835037000000	-0.437235000000
H	-1.081495000000	-3.152317000000	-1.161885000000
H	0.678026000000	-3.061909000000	-0.770383000000
C	0.579335000000	2.029784000000	0.232859000000
H	0.705982000000	2.604035000000	-0.686791000000
H	-0.069154000000	2.577844000000	0.917163000000
H	1.540142000000	1.876141000000	0.714296000000
H	-0.529711000000	-3.311165000000	0.525433000000
N	-5.277979000000	4.742989000000	0.394605000000
H	-5.754567000000	4.811748000000	1.287915000000
H	-5.000604000000	5.653007000000	0.041410000000
N	-6.768824000000	-3.247783000000	-0.537322000000
H	-7.223520000000	-3.203727000000	-1.443620000000
H	-6.846222000000	-4.169930000000	-0.120682000000

TS4 neutral singlet, imaginary frequency = 118.6*i* cm^{-1}

C	2.528881000000	-0.735900000000	0.347993000000
O	2.492204000000	-1.784024000000	1.029058000000
C	2.466611000000	0.590541000000	1.072437000000
C	3.219166000000	1.704460000000	0.694701000000
C	1.617626000000	0.687760000000	2.181724000000
C	3.128023000000	2.896800000000	1.418634000000
H	3.874973000000	1.663011000000	-0.169243000000
C	1.509588000000	1.879023000000	2.891357000000
C	2.271592000000	2.989864000000	2.512774000000
H	3.723606000000	3.754285000000	1.117651000000
H	0.833752000000	1.945048000000	3.739798000000
H	2.193713000000	3.920448000000	3.068269000000
H	1.025893000000	-0.179356000000	2.466449000000
C	7.576241000000	-0.390231000000	-0.529231000000
C	6.892242000000	0.321780000000	-1.514457000000
C	5.510061000000	0.179408000000	-1.644662000000
C	4.794502000000	-0.669962000000	-0.795808000000
C	5.489787000000	-1.386443000000	0.185605000000
C	6.870643000000	-1.245955000000	0.319033000000
H	8.652045000000	-0.280314000000	-0.422751000000
H	7.433541000000	0.987015000000	-2.182035000000
H	4.978400000000	0.738281000000	-2.412803000000

H	4.946078000000	-2.052786000000	0.850351000000
H	7.397148000000	-1.803217000000	1.089295000000
C	3.291408000000	-0.836301000000	-0.989773000000
O	3.015403000000	-2.108172000000	-1.547683000000
H	2.937526000000	-0.074927000000	-1.690429000000
H	2.829085000000	-2.680720000000	-0.777951000000
N	-0.183865000000	0.611191000000	-0.632097000000
C	0.513376000000	-0.538973000000	-0.475217000000
C	-1.551035000000	0.418841000000	-0.455880000000
C	-1.712718000000	-0.913893000000	-0.191374000000
N	-0.433908000000	-1.467225000000	-0.206936000000
C	-2.949256000000	-1.663172000000	0.086414000000
C	-3.841520000000	-1.209117000000	1.067610000000
C	-3.291592000000	-2.815292000000	-0.635092000000
C	-5.033311000000	-1.876933000000	1.321295000000
C	-4.476943000000	-3.495686000000	-0.381490000000
C	-5.368311000000	-3.035504000000	0.601601000000
H	-3.594835000000	-0.320554000000	1.644232000000
H	-2.626787000000	-3.182613000000	-1.413501000000
H	-5.712871000000	-1.508758000000	2.086226000000
H	-4.726508000000	-4.387419000000	-0.951636000000
C	-2.570872000000	1.470515000000	-0.596904000000
C	-3.691728000000	1.257087000000	-1.411772000000
C	-2.480231000000	2.686828000000	0.094201000000
C	-4.689205000000	2.216686000000	-1.531012000000
C	-3.468599000000	3.657156000000	-0.026608000000
C	-4.591536000000	3.435889000000	-0.840418000000
H	-3.781595000000	0.324112000000	-1.963556000000
H	-1.631350000000	2.876132000000	0.747802000000
H	-5.550687000000	2.031368000000	-2.168442000000
H	-3.381625000000	4.593942000000	0.518815000000
C	-0.148351000000	-2.881389000000	0.006851000000
H	0.854691000000	-2.970582000000	0.420540000000
H	-0.870631000000	-3.293526000000	0.713853000000
C	0.425300000000	1.884848000000	-0.988491000000
H	1.390171000000	1.687423000000	-1.455381000000
H	-0.218377000000	2.406120000000	-1.700521000000
H	0.571321000000	2.510022000000	-0.102440000000
H	-0.214927000000	-3.428770000000	-0.937407000000
N	-5.614540000000	4.375566000000	-0.910581000000
H	-5.333456000000	5.330492000000	-0.711929000000
H	-6.187211000000	4.321827000000	-1.746803000000
N	-6.584537000000	-3.676493000000	0.813289000000
H	-6.601321000000	-4.657005000000	0.551336000000
H	-6.991700000000	-3.529090000000	1.731255000000

4,5-bis(p-cyanophenyl)-1,3-dimethylimidazolylidene

Carbene neutral singlet

N	-1.064270000000	2.901500000000	0.025957000000
C	0.000039000000	3.746208000000	-0.000030000000
C	-0.684223000000	1.565383000000	0.013468000000
C	0.684208000000	1.565359000000	-0.013536000000
N	1.064312000000	2.901455000000	-0.025974000000
C	1.610883000000	0.422761000000	-0.053253000000
C	2.686082000000	0.335795000000	0.842679000000
C	1.402424000000	-0.609112000000	-0.980595000000
C	3.542471000000	-0.757570000000	0.813456000000
C	2.247187000000	-1.710804000000	-1.014162000000
C	3.319846000000	-1.780563000000	-0.116231000000
H	2.843025000000	1.114912000000	1.582311000000
H	0.577418000000	-0.542637000000	-1.684217000000
H	4.371888000000	-0.826091000000	1.510058000000
H	2.086780000000	-2.507740000000	-1.733360000000
C	-1.610918000000	0.422800000000	0.053215000000
C	-2.686070000000	0.335762000000	-0.842771000000
C	-1.402489000000	-0.609025000000	0.980619000000
C	-3.542451000000	-0.757607000000	-0.813521000000
C	-2.247250000000	-1.710719000000	1.014217000000
C	-3.319869000000	-1.780537000000	0.116244000000
H	-2.842970000000	1.114812000000	-1.582480000000
H	-0.577514000000	-0.542506000000	1.684272000000
H	-4.371828000000	-0.826182000000	-1.510166000000
H	-2.086869000000	-2.507611000000	1.733470000000
C	2.442614000000	3.369640000000	-0.106289000000
H	2.423802000000	4.407735000000	-0.436843000000
H	2.933266000000	3.311888000000	0.868244000000
C	-2.442538000000	3.369770000000	0.106370000000
H	-2.933229000000	3.312163000000	-0.868151000000
H	-2.999055000000	2.770579000000	0.830357000000
H	-2.423640000000	4.407830000000	0.437032000000
H	2.999110000000	2.770480000000	-0.830318000000
C	4.202652000000	-2.915180000000	-0.149243000000
N	4.914139000000	-3.828689000000	-0.175948000000
C	-4.202667000000	-2.915159000000	0.149281000000
N	-4.914148000000	-3.828673000000	0.176006000000

TS1 neutral singlet, imaginary frequency = 218.1*i* cm^{-1}

C	3.470490000000	-2.076445000000	0.368252000000
O	3.179592000000	-2.473271000000	1.515182000000
C	4.474856000000	-0.972576000000	0.158866000000
C	5.084820000000	-0.815003000000	-1.087440000000

C	4.807758000000	-0.113045000000	1.205862000000
C	6.001866000000	0.213973000000	-1.296658000000
H	4.824254000000	-1.491398000000	-1.900430000000
C	5.720851000000	0.920649000000	0.998966000000
C	6.315708000000	1.089051000000	-0.253647000000
H	6.471030000000	0.335686000000	-2.269304000000
H	5.970209000000	1.595678000000	1.813512000000
H	7.027740000000	1.893872000000	-0.414581000000
H	4.334431000000	-0.254069000000	2.174370000000
H	3.446969000000	-2.782747000000	-0.482021000000
N	1.338743000000	0.193175000000	-0.290241000000
C	1.736930000000	-1.099492000000	-0.319897000000
C	-0.043179000000	0.296043000000	-0.169240000000
C	-0.518699000000	-0.986885000000	-0.133504000000
N	0.593320000000	-1.812901000000	-0.218877000000
C	-1.908604000000	-1.461120000000	-0.036990000000
C	-2.756773000000	-0.941122000000	0.950338000000
C	-2.403361000000	-2.405095000000	-0.948032000000
C	-4.081143000000	-1.351722000000	1.028303000000
C	-3.724383000000	-2.827471000000	-0.875648000000
C	-4.561468000000	-2.297116000000	0.113421000000
H	-2.373583000000	-0.217524000000	1.664298000000
H	-1.757194000000	-2.799338000000	-1.727455000000
H	-4.739430000000	-0.951091000000	1.792708000000
H	-4.110503000000	-3.554414000000	-1.582934000000
C	-0.790378000000	1.563415000000	-0.133180000000
C	-1.903712000000	1.734540000000	-0.968351000000
C	-0.421094000000	2.591894000000	0.744911000000
C	-2.642953000000	2.909261000000	-0.926944000000
C	-1.148990000000	3.774286000000	0.789762000000
C	-2.261126000000	3.928912000000	-0.046470000000
H	-2.187158000000	0.944733000000	-1.658230000000
H	0.427420000000	2.461136000000	1.410074000000
H	-3.504303000000	3.042504000000	-1.573980000000
H	-0.866492000000	4.569664000000	1.472119000000
C	0.562226000000	-3.271836000000	-0.150450000000
H	0.488816000000	-3.700575000000	-1.152656000000
H	1.472974000000	-3.610013000000	0.343485000000
C	2.234625000000	1.337317000000	-0.447779000000
H	1.734927000000	2.104111000000	-1.042933000000
H	2.507843000000	1.751266000000	0.525587000000
H	3.131568000000	1.008111000000	-0.970748000000
H	-0.297747000000	-3.585611000000	0.443142000000
C	-3.022415000000	5.148293000000	0.002562000000
N	-3.636298000000	6.129389000000	0.044937000000
C	-5.931793000000	-2.727253000000	0.188779000000
N	-7.035605000000	-3.072882000000	0.247006000000

INT1 neutral singlet

C	-3.305104000000	-1.040571000000	-1.223269000000
O	-3.589645000000	-0.491956000000	-2.412654000000
C	-4.201173000000	-0.593606000000	-0.042671000000
C	-3.988096000000	-1.069506000000	1.256630000000
C	-5.258420000000	0.282879000000	-0.278167000000
C	-4.816376000000	-0.670126000000	2.304641000000
H	-3.165569000000	-1.758705000000	1.450871000000
C	-6.093108000000	0.685571000000	0.768259000000
C	-5.873845000000	0.211736000000	2.062014000000
H	-4.640106000000	-1.045121000000	3.309520000000
H	-6.914797000000	1.370408000000	0.573681000000
H	-6.520878000000	0.524622000000	2.876978000000
H	-5.406142000000	0.638925000000	-1.294366000000
H	-3.353797000000	-2.152822000000	-1.213293000000
N	-0.857351000000	-1.602875000000	-0.578713000000
C	-1.850989000000	-0.731858000000	-0.812743000000
C	0.324575000000	-0.908386000000	-0.354074000000
C	0.017954000000	0.423417000000	-0.442901000000
N	-1.334860000000	0.501796000000	-0.728428000000
C	0.899684000000	1.592834000000	-0.295478000000
C	0.554509000000	2.640211000000	0.568870000000
C	2.110373000000	1.640658000000	-0.999534000000
C	1.405906000000	3.725967000000	0.729192000000
C	2.971935000000	2.718445000000	-0.841093000000
C	2.615001000000	3.759960000000	0.024079000000
H	-0.372359000000	2.599986000000	1.133225000000
H	2.374279000000	0.834016000000	-1.677478000000
H	1.143948000000	4.536988000000	1.400871000000
H	3.909670000000	2.759923000000	-1.385641000000
C	1.621448000000	-1.542787000000	-0.070236000000
C	2.115598000000	-2.561848000000	-0.895759000000
C	2.383705000000	-1.097509000000	1.018249000000
C	3.354585000000	-3.134536000000	-0.637508000000
C	3.627025000000	-1.657591000000	1.280292000000
C	4.108171000000	-2.677693000000	0.450573000000
H	1.537176000000	-2.898510000000	-1.751509000000
H	1.997333000000	-0.315397000000	1.665595000000
H	3.741761000000	-3.922410000000	-1.275512000000
H	4.218960000000	-1.316612000000	2.123572000000
C	-2.103922000000	1.726046000000	-0.958810000000
H	-2.924875000000	1.462095000000	-1.627456000000
H	-2.481044000000	2.113184000000	-0.009321000000
C	-1.015470000000	-3.057005000000	-0.498696000000
H	-0.985966000000	-3.494081000000	-1.498886000000
H	-0.204708000000	-3.460063000000	0.107046000000

H	-1.962543000000	-3.289773000000	-0.014432000000
H	-1.453804000000	2.464823000000	-1.429449000000
C	3.502854000000	4.879708000000	0.190867000000
N	4.217752000000	5.780605000000	0.325549000000
C	5.393610000000	-3.264347000000	0.720651000000
N	6.428463000000	-3.736127000000	0.938297000000

TS2 neutral singlet, imaginary frequency = 1217.3*i* cm^{-1}

C	-3.116002000000	0.010405000000	0.649906000000
C	-3.846289000000	-0.313067000000	-0.603970000000
C	-5.106213000000	-0.935167000000	-0.550925000000
C	-3.359014000000	0.072673000000	-1.868745000000
C	-5.845218000000	-1.160423000000	-1.712549000000
H	-5.496833000000	-1.246626000000	0.412900000000
C	-4.101830000000	-0.151318000000	-3.025386000000
C	-5.352922000000	-0.769597000000	-2.958437000000
H	-6.814954000000	-1.647380000000	-1.640313000000
H	-3.698265000000	0.157683000000	-3.986545000000
H	-5.929580000000	-0.947101000000	-3.861769000000
H	-2.386166000000	0.554855000000	-1.955013000000
H	-3.639220000000	1.274419000000	1.022966000000
O	-3.492312000000	-0.851253000000	1.725250000000
H	-3.572222000000	-0.296600000000	2.529717000000
O	-3.635886000000	1.068279000000	3.757114000000
O	-4.185704000000	2.248181000000	1.491579000000
H	-3.925815000000	1.665594000000	3.000402000000
H	-4.372876000000	1.032917000000	4.384622000000
H	-5.126871000000	2.168030000000	1.270136000000
N	-0.852876000000	1.061882000000	0.263724000000
C	-1.639269000000	-0.011138000000	0.469512000000
C	0.467106000000	0.660794000000	0.148078000000
C	0.478373000000	-0.702089000000	0.286922000000
N	-0.835843000000	-1.093064000000	0.473163000000
C	1.633780000000	-1.616248000000	0.278156000000
C	1.657967000000	-2.745300000000	-0.551109000000
C	2.742792000000	-1.320652000000	1.082738000000
C	2.772512000000	-3.574464000000	-0.573545000000
C	3.864945000000	-2.138354000000	1.061967000000
C	3.874590000000	-3.266322000000	0.232514000000
H	0.813859000000	-2.970120000000	-1.195933000000
H	2.724677000000	-0.448728000000	1.730276000000
H	2.794830000000	-4.448022000000	-1.216971000000
H	4.724852000000	-1.910811000000	1.683867000000
C	1.595935000000	1.572004000000	-0.107208000000
C	1.801019000000	2.709027000000	0.684761000000
C	2.494460000000	1.270602000000	-1.139671000000

C	2.889074000000	3.540090000000	0.448452000000
C	3.588683000000	2.090695000000	-1.379958000000
C	3.781162000000	3.226191000000	-0.583924000000
H	1.120170000000	2.936945000000	1.499376000000
H	2.329858000000	0.394359000000	-1.760684000000
H	3.054374000000	4.420440000000	1.061561000000
H	4.285139000000	1.862384000000	-2.180434000000
C	-1.304811000000	-2.475538000000	0.578227000000
H	-2.260327000000	-2.471915000000	1.097585000000
H	-1.418030000000	-2.899492000000	-0.422221000000
C	-1.327910000000	2.438834000000	0.117955000000
H	-2.377778000000	2.424480000000	-0.166294000000
H	-1.217458000000	2.973745000000	1.063406000000
H	-0.741443000000	2.927035000000	-0.661619000000
H	-0.575854000000	-3.054068000000	1.147542000000
C	4.910627000000	4.082381000000	-0.832639000000
N	5.819596000000	4.771043000000	-1.033349000000
C	5.033622000000	-4.118103000000	0.206063000000
N	5.968289000000	-4.801170000000	0.183433000000

BINT neutral singlet

C	-3.064515000000	-1.359176000000	-0.339116000000
O	-3.235860000000	-2.642581000000	-0.868289000000
C	-4.255991000000	-0.607526000000	0.007425000000
C	-4.235239000000	0.481819000000	0.910203000000
C	-5.515547000000	-1.007994000000	-0.492493000000
C	-5.401872000000	1.155877000000	1.252534000000
H	-3.295734000000	0.781801000000	1.368204000000
C	-6.680847000000	-0.331844000000	-0.137985000000
C	-6.637918000000	0.760895000000	0.730025000000
H	-5.348503000000	1.987936000000	1.950467000000
H	-7.632057000000	-0.662088000000	-0.548373000000
H	-7.547458000000	1.287268000000	1.004147000000
H	-5.570311000000	-1.848914000000	-1.177707000000
H	-3.691573000000	-3.203393000000	-0.216576000000
N	-1.293838000000	0.382691000000	-0.303466000000
C	-1.758796000000	-0.921187000000	-0.246938000000
C	0.102119000000	0.369251000000	-0.183905000000
C	0.498473000000	-0.930090000000	-0.078683000000
N	-0.643732000000	-1.731925000000	-0.126894000000
C	1.847148000000	-1.489115000000	0.061246000000
C	2.229866000000	-2.598400000000	-0.709185000000
C	2.765904000000	-0.920901000000	0.956563000000
C	3.510940000000	-3.121966000000	-0.602967000000
C	4.051186000000	-1.433168000000	1.065986000000
C	4.422932000000	-2.534643000000	0.283859000000

H	1.524025000000	-3.044216000000	-1.404844000000
H	2.468218000000	-0.080051000000	1.576199000000
H	3.809414000000	-3.975268000000	-1.203629000000
H	4.761728000000	-0.994057000000	1.759041000000
C	0.893925000000	1.601646000000	-0.190671000000
C	0.449749000000	2.720105000000	0.533619000000
C	2.096458000000	1.682253000000	-0.910701000000
C	1.196976000000	3.889074000000	0.556033000000
C	2.854488000000	2.844445000000	-0.888808000000
C	2.403820000000	3.949123000000	-0.153502000000
H	-0.478209000000	2.667149000000	1.096388000000
H	2.432950000000	0.833915000000	-1.499365000000
H	0.856114000000	4.749566000000	1.122986000000
H	3.783486000000	2.905962000000	-1.446707000000
C	-0.724738000000	-3.078476000000	0.423580000000
H	-1.535582000000	-3.112923000000	1.157912000000
H	-0.914909000000	-3.818282000000	-0.356139000000
C	-2.016103000000	1.447076000000	-0.986525000000
H	-2.514200000000	2.123313000000	-0.286011000000
H	-1.316014000000	2.017972000000	-1.599847000000
H	-2.770385000000	0.993213000000	-1.634680000000
H	0.213198000000	-3.313213000000	0.928085000000
C	5.750888000000	-3.072126000000	0.397676000000
N	6.821719000000	-3.504625000000	0.488405000000
C	3.182275000000	5.156717000000	-0.132457000000
N	3.810019000000	6.130280000000	-0.114062000000

TS3 neutral singlet, imaginary frequency = 212.6*i* cm^{-1}

C	1.231718000000	0.561922000000	-0.511975000000
C	1.433454000000	-0.786341000000	-0.481316000000
C	-0.730862000000	-0.434204000000	-0.969920000000
N	0.216521000000	-1.388878000000	-0.768170000000
N	-0.101309000000	0.768058000000	-0.851908000000
C	-2.139007000000	-0.694015000000	-1.210833000000
O	-2.344244000000	-1.629244000000	-2.203760000000
H	-2.801374000000	-2.398984000000	-1.739062000000
C	-2.759878000000	-2.070858000000	0.438194000000
O	-3.149379000000	-3.028247000000	-0.302782000000
H	-1.752952000000	-2.107154000000	0.889942000000
C	-3.730302000000	-1.300221000000	1.255346000000
C	-5.086712000000	-1.257794000000	0.908235000000
C	-3.290889000000	-0.610284000000	2.388700000000
C	-5.983938000000	-0.517482000000	1.673710000000
C	-4.190460000000	0.118545000000	3.166748000000
C	-5.537536000000	0.172843000000	2.805554000000
H	-5.423293000000	-1.804986000000	0.031382000000

H	-2.235668000000	-0.641726000000	2.656655000000
H	-7.033379000000	-0.478626000000	1.393045000000
H	-3.841704000000	0.648060000000	4.049467000000
H	-6.239076000000	0.747188000000	3.404703000000
C	-3.139458000000	0.384136000000	-1.124616000000
C	-4.241482000000	0.388781000000	-1.995169000000
C	-3.116145000000	1.348789000000	-0.096379000000
C	-5.265300000000	1.329177000000	-1.856971000000
C	-4.131292000000	2.286683000000	0.036393000000
C	-5.219596000000	2.285267000000	-0.844126000000
H	-4.292321000000	-0.356151000000	-2.783367000000
H	-2.301229000000	1.348559000000	0.624216000000
H	-6.104426000000	1.308632000000	-2.548316000000
H	-4.084639000000	3.014228000000	0.843565000000
H	-6.016963000000	3.015080000000	-0.734924000000
C	0.044945000000	-2.839761000000	-0.860538000000
H	-1.004464000000	-3.104239000000	-0.774330000000
H	0.417801000000	-3.191407000000	-1.825349000000
H	0.607530000000	-3.310073000000	-0.052144000000
C	-0.558279000000	2.034287000000	-1.435486000000
H	-0.966584000000	2.704691000000	-0.678479000000
H	0.299327000000	2.505013000000	-1.918365000000
H	-1.316926000000	1.825655000000	-2.187611000000
C	2.178500000000	1.657321000000	-0.266532000000
C	1.799715000000	2.754079000000	0.521121000000
C	3.470777000000	1.604954000000	-0.808062000000
C	2.696783000000	3.784190000000	0.769338000000
C	4.377792000000	2.626208000000	-0.559090000000
C	3.987092000000	3.715886000000	0.229229000000
H	0.803798000000	2.795424000000	0.953104000000
H	3.762764000000	0.767801000000	-1.435554000000
H	2.406596000000	4.632439000000	1.380995000000
H	5.378349000000	2.588625000000	-0.977997000000
C	2.667004000000	-1.522913000000	-0.153768000000
C	3.337992000000	-1.236000000000	1.042486000000
C	3.199702000000	-2.467783000000	-1.040813000000
C	4.528510000000	-1.880746000000	1.352251000000
C	4.385539000000	-3.123786000000	-0.737144000000
C	5.047873000000	-2.826501000000	0.460076000000
H	2.923181000000	-0.507233000000	1.733188000000
H	2.699487000000	-2.676053000000	-1.981641000000
H	5.050333000000	-1.660478000000	2.278154000000
H	4.803531000000	-3.852011000000	-1.424659000000
C	6.279559000000	-3.498477000000	0.777273000000
N	7.272013000000	-4.036705000000	1.034527000000
C	4.920938000000	4.779564000000	0.483913000000
N	5.671455000000	5.636793000000	0.691374000000

INT2 neutral singlet

C	2.331798000000	-0.784472000000	-0.211131000000
O	2.554859000000	-2.050323000000	-0.605216000000
C	2.827871000000	-0.535147000000	1.232439000000
C	3.549571000000	0.580504000000	1.667214000000
C	2.527378000000	-1.536030000000	2.167006000000
C	3.963776000000	0.691231000000	2.998470000000
H	3.808689000000	1.376520000000	0.975746000000
C	2.928841000000	-1.426469000000	3.495799000000
C	3.654983000000	-0.309159000000	3.917187000000
H	4.531913000000	1.563412000000	3.310757000000
H	2.682222000000	-2.214334000000	4.202620000000
H	3.977999000000	-0.222709000000	4.950935000000
H	1.983578000000	-2.414870000000	1.828899000000
C	7.249455000000	0.562232000000	-1.302844000000
C	6.431904000000	1.688833000000	-1.387652000000
C	5.043312000000	1.543172000000	-1.382683000000
C	4.450787000000	0.279688000000	-1.291289000000
C	5.280276000000	-0.847518000000	-1.217078000000
C	6.667712000000	-0.705239000000	-1.218715000000
H	8.330776000000	0.669176000000	-1.305225000000
H	6.872163000000	2.679942000000	-1.458005000000
H	4.409015000000	2.426287000000	-1.441148000000
H	4.820806000000	-1.828629000000	-1.142536000000
H	7.299345000000	-1.587557000000	-1.154138000000
C	2.936013000000	0.166202000000	-1.325698000000
O	2.510225000000	-0.418319000000	-2.546634000000
H	2.528045000000	1.178845000000	-1.294058000000
H	2.493257000000	-1.376389000000	-2.293661000000
N	0.165144000000	0.709818000000	-0.051081000000
C	0.777431000000	-0.488749000000	-0.175465000000
C	-1.209501000000	0.541418000000	-0.068744000000
C	-1.437616000000	-0.797918000000	-0.186426000000
N	-0.198154000000	-1.415567000000	-0.256529000000
C	-2.731613000000	-1.500038000000	-0.261748000000
C	-3.045003000000	-2.528931000000	0.636043000000
C	-3.675806000000	-1.093363000000	-1.213318000000
C	-4.285246000000	-3.151948000000	0.581763000000
C	-4.921633000000	-1.705536000000	-1.272543000000
C	-5.220816000000	-2.736407000000	-0.374063000000
H	-2.324787000000	-2.833244000000	1.389438000000
H	-3.431055000000	-0.297570000000	-1.911134000000
H	-4.533783000000	-3.947153000000	1.277075000000
H	-5.655279000000	-1.394492000000	-2.009148000000
C	-2.187843000000	1.637685000000	0.030768000000

C	-2.125060000000	2.735465000000	-0.837820000000
C	-3.216358000000	1.556010000000	0.978476000000
C	-3.076216000000	3.744686000000	-0.760125000000
C	-4.176163000000	2.556940000000	1.060561000000
C	-4.100829000000	3.650467000000	0.189737000000
H	-1.340937000000	2.794009000000	-1.587438000000
H	-3.260109000000	0.708784000000	1.656990000000
H	-3.034697000000	4.594678000000	-1.433573000000
H	-4.973970000000	2.498316000000	1.793984000000
C	-0.075462000000	-2.873736000000	-0.415340000000
H	-0.885743000000	-3.207209000000	-1.064593000000
H	0.900100000000	-3.083181000000	-0.840293000000
C	0.783609000000	2.014524000000	0.200223000000
H	0.909103000000	2.565314000000	-0.733551000000
H	0.130630000000	2.572943000000	0.871592000000
H	1.743409000000	1.877979000000	0.688378000000
H	-0.167897000000	-3.350745000000	0.562887000000
C	-5.090709000000	4.691577000000	0.269006000000
N	-5.887056000000	5.529796000000	0.331854000000
C	-6.508581000000	-3.375856000000	-0.431468000000
N	-7.544939000000	-3.890289000000	-0.476993000000

TS4 neutral singlet, imaginary frequency = 128.8*i* cm^{-1}

C	2.738324000000	-0.741191000000	0.354273000000
O	2.732532000000	-1.811925000000	1.006368000000
C	2.737801000000	0.559859000000	1.129596000000
C	3.465296000000	1.685663000000	0.738211000000
C	1.980328000000	0.615253000000	2.305595000000
C	3.435635000000	2.849871000000	1.511284000000
H	4.053745000000	1.675288000000	-0.173995000000
C	1.933815000000	1.778691000000	3.067029000000
C	2.667370000000	2.902326000000	2.671917000000
H	4.011080000000	3.716813000000	1.198372000000
H	1.330021000000	1.811363000000	3.969904000000
H	2.638614000000	3.810504000000	3.267566000000
H	1.415411000000	-0.263650000000	2.607226000000
C	7.757956000000	-0.437349000000	-0.707985000000
C	7.045041000000	0.336968000000	-1.623111000000
C	5.656503000000	0.220509000000	-1.702012000000
C	4.963276000000	-0.664891000000	-0.871757000000
C	5.687392000000	-1.443430000000	0.039084000000
C	7.074625000000	-1.328983000000	0.121197000000
H	8.838899000000	-0.348618000000	-0.641877000000
H	7.567826000000	1.031107000000	-2.275832000000
H	5.101975000000	0.828308000000	-2.415068000000
H	5.161372000000	-2.139179000000	0.687803000000

H	7.624443000000	-1.936192000000	0.835491000000
C	3.452030000000	-0.805607000000	-1.013604000000
O	3.136325000000	-2.055914000000	-1.599600000000
H	3.084246000000	-0.018799000000	-1.678554000000
H	2.997593000000	-2.655251000000	-0.839966000000
N	0.032837000000	0.630559000000	-0.520966000000
C	0.733483000000	-0.518587000000	-0.374963000000
C	-1.332498000000	0.417471000000	-0.396221000000
C	-1.489656000000	-0.923810000000	-0.178340000000
N	-0.209681000000	-1.465527000000	-0.166455000000
C	-2.733064000000	-1.680541000000	0.041409000000
C	-3.667039000000	-1.205037000000	0.973579000000
C	-3.015507000000	-2.844980000000	-0.686430000000
C	-4.867533000000	-1.872829000000	1.174427000000
C	-4.209549000000	-3.526377000000	-0.487261000000
C	-5.135274000000	-3.035908000000	0.442129000000
H	-3.445674000000	-0.311381000000	1.550268000000
H	-2.307390000000	-3.213259000000	-1.422926000000
H	-5.589491000000	-1.503867000000	1.895971000000
H	-4.431557000000	-4.425712000000	-1.053030000000
C	-2.359665000000	1.463940000000	-0.525909000000
C	-3.443662000000	1.261508000000	-1.391372000000
C	-2.286164000000	2.643958000000	0.227151000000
C	-4.445052000000	2.217130000000	-1.503287000000
C	-3.279291000000	3.609419000000	0.119034000000
C	-4.357761000000	3.392219000000	-0.746993000000
H	-3.497508000000	0.353228000000	-1.984869000000
H	-1.460801000000	2.800536000000	0.916259000000
H	-5.283472000000	2.062367000000	-2.175130000000
H	-3.227854000000	4.520956000000	0.705874000000
C	0.082965000000	-2.882725000000	0.033129000000
H	1.080010000000	-2.967020000000	0.461027000000
H	-0.646297000000	-3.308055000000	0.724897000000
C	0.637073000000	1.918715000000	-0.841273000000
H	1.602079000000	1.738415000000	-1.313451000000
H	-0.008249000000	2.454681000000	-1.540303000000
H	0.778193000000	2.516811000000	0.063459000000
H	0.035061000000	-3.415059000000	-0.920193000000
C	-5.387138000000	4.390352000000	-0.861036000000
N	-6.215128000000	5.195220000000	-0.949323000000
C	-6.375259000000	-3.735343000000	0.645723000000
N	-7.374019000000	-4.298710000000	0.807838000000