

Supporting Information

for the article

Adaptive Carbonyl Umpolung Involving Carbanionic Carbene Breslow Intermediate: An Alternative Mechanism for NHC-mediated Organocatalysis

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1. Experimental Part.

1.1. General Information.

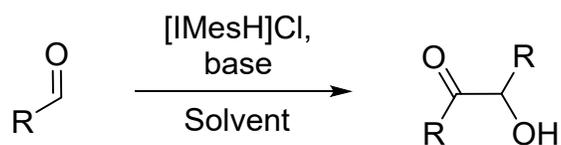
Commercially available starting compounds, reagents and solvents were of analytical grade. Imidazolium salts were obtained by using published synthetic protocols or purchased commercially. NMR spectra were recorded using a Bruker Avance 300 spectrometer operating at 300.1 MHz for ^1H and 75.5 MHz for ^{13}C . NMR chemical shifts were measured relative to residual solvent peaks. The processing was carried out using the MestReNova software.

1.2. Mechanistic experiments.

We conducted a comparative experimental study on the catalytic activity of 1,3-bis(2,4,6-trimethylphenyl)-imidazol-2-ylidene (IMes) and 1,3-bis(2,6-diisopropylphenyl)-imidazol-2-ylidene (IPr) in the benzoin condensation reaction with various aromatic aldehydes and isobutyraldehyde. The results of these experiments are presented in Tables S1 and S2. The NHCs were generated *in situ* in the H-bonded form by deprotonating the appropriate imidazolium cations with DBU or sodium *tert*-butoxide, following previously reported methods.^[1] The best selectivity was observed for the reactions with furaldehydes under ambient conditions for 24 hours. In contrast, benzaldehydes exhibited lower reactivity (Table S1, entries 6-9; Table S2, entries 6-8), and isobutyraldehyde was almost inactive (Table S1, entry 10; Table S2, entry 9). Additionally, we investigated the influence of solvent on the selectivity of the benzoin condensation of furfural. The best results were obtained when using THF and methanol as solvents, while the reactions conducted under solvent-free conditions showed the lowest efficiency (Table S1, entries 11-16; Table S2, entries 10-16).

General procedure for benzoin condensation. A mixture of aldehyde (0.5 mmol), imidazolium chloride (0.05 mmol) and a base (0.5 mmol) in deuterated solvent was treated at the appropriate temperature and time conditions (24 h at 22 °C or 3 h at 80 °C) under an argon atmosphere. The degree of conversion and the yield of benzoin condensation products were measured by NMR using DBU or PhSiMe₃ as internal standard.

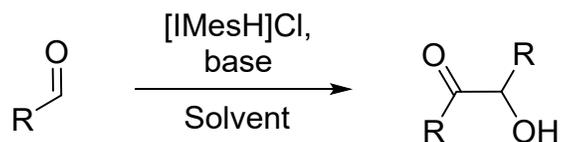
Table S1. Catalytic activity of [IMesH]⁺ in benzoin condensation of aldehydes.



Entry	Imidazolium salt, base	Solvent	Aldehyde	T (°C)	Conversion/yield (%)
1	[IMesH]Cl, DBU	CD ₃ CN	Furfural	22 °C	98/51
2	[IMesH]Cl, DBU	CD ₃ CN	Furfural	80 °C	96/41
3 ^a	[IMesH]Cl, DBU	CD ₃ CN	Furfural	22 °C	96/45
4	[IMesH]Cl, ^t BuONa	CD ₃ CN	Furfural	22 °C	99/32
5	[IMesH]Cl, DBU	CD ₃ CN	5-Methylfurfural	22 °C	93/63
6	[IMesH]Cl, DBU	CD ₃ CN	Benzaldehyde	22 °C	23/18
7	[IMesH]Cl, DBU	CD ₃ CN	Benzaldehyde	80 °C	77/24
8	[IMesH]Cl, DBU	CD ₃ CN	<i>m</i> -Anisaldehyde	80 °C	84/41
9 ^a	[IMesH]Cl, DBU	CD ₃ CN	<i>m</i> -Anisaldehyde	80 °C	84/47
10	[IMesH]Cl, DBU	CD ₃ CN	Isobutyraldehyde	80 °C	38/8
11	[IMesH]Cl, DBU	CDCl ₃	Furfural	22 °C	96/73
12	[IMesH]Cl, DBU	THF- <i>d</i> ₈	Furfural	22 °C	96/90
13	[IMesH]Cl, DBU	Neat	Furfural	22 °C	80/20
14	[IMesH]Cl, ^t BuONa	CD ₃ OD	Furfural	22 °C	100/77
15	[IMesH]Cl, ^t BuONa	THF- <i>d</i> ₈	Furfural	22 °C	97/70
16	[IMesH]Cl, ^t BuONa	Neat	Furfural	22 °C	34/5

^a 0.1 mmol of a base was used.

Table S2. Catalytic activity of [PrH]⁺ in benzoin condensation of aldehydes.



Entry	Imidazolium salt, base	Solvent	Aldehyde	T (°C)	Conversion/yield (%)
1	[IPrH]Cl, DBU	CD ₃ CN	Furfural	22 °C	99/40
2 ^a	[IPrH]Cl, DBU	CD ₃ CN	Furfural	22 °C	99/33
3	[IPrH]Cl, DBU	CD ₃ CN	Furfural	80 °C	99/38
4	[IPrH]Cl, ^t BuONa	CD ₃ CN	Furfural	22 °C	99/34
5	[IPrH]Cl, DBU	CD ₃ CN	5-Methylfurfural	22 °C	93/53
6	[IPrH]Cl, DBU	CD ₃ CN	Benzaldehyde	80 °C	53/5
7	[IPrH]Cl, DBU	CD ₃ CN	<i>m</i> -Anisaldehyde	80 °C	31/14
8 ^a	[IPrH]Cl, DBU	CD ₃ CN	<i>m</i> -Anisaldehyde	80 °C	46/20
9	[IPrH]Cl, DBU	CD ₃ CN	Isobutyraldehyde	80 °C	31/2
10	[IPrH]Cl, DBU	CD ₃ OD	Furfural	22 °C	100/71
11	[IPrH]Cl, DBU	CDCl ₃	Furfural	22 °C	95/56
12	[IPrH]Cl, DBU	THF- <i>d</i> ₈	Furfural	22 °C	98/82
13	[IPrH]Cl, DBU	Neat	Furfural	22 °C	79/18
14	[IPrH]Cl, ^t BuONa	CD ₃ OD	Furfural	22 °C	100/94
15	[IPrH]Cl, ^t BuONa	THF- <i>d</i> ₈	Furfural	22 °C	97/83
16	[IPrH]Cl, ^t BuONa	Neat	Furfural	22 °C	51/10

^a 0.1 mmol of a base was used.

[1] (a) K. I. Galkin and V. P. Ananikov, Towards Improved Biorefinery Technologies: 5-Methylfurfural as a Versatile C(6) Platform for Biofuels Development, *ChemSusChem*, 2019, **12**, 185-189; (b) R. S. Menon, A. T. Biju and V. Nair, Recent advances in N-heterocyclic carbene (NHC)-catalysed benzoin reactions, *Beilstein J. Org. Chem.*, 2016, **12**, 444-461.

1.3. Selected NMR spectra of reaction mixtures.

Figure S1. ^1H NMR spectra of the reaction mixture (conditions from entry 4, Table S1).

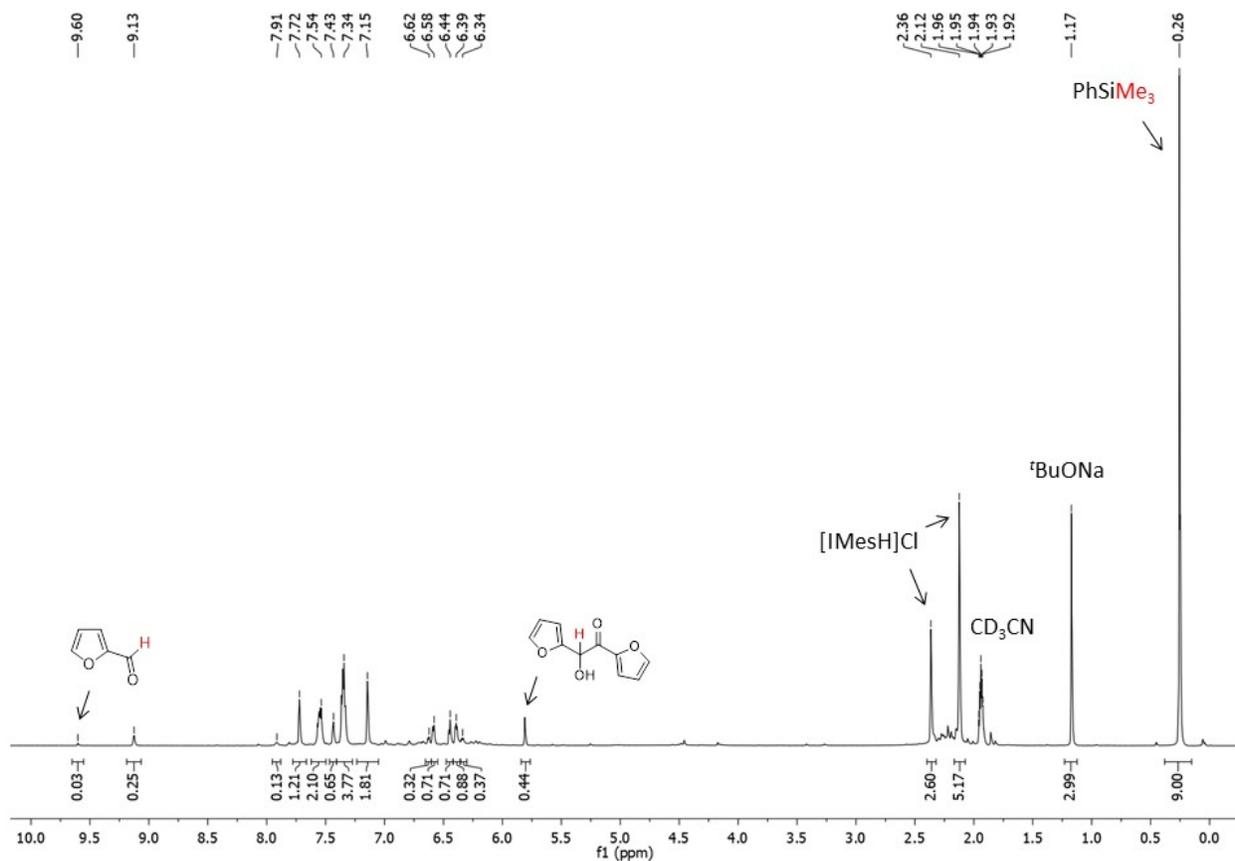


Figure S2. ^1H NMR spectra of the reaction mixture (conditions from entry 5, Table S1).

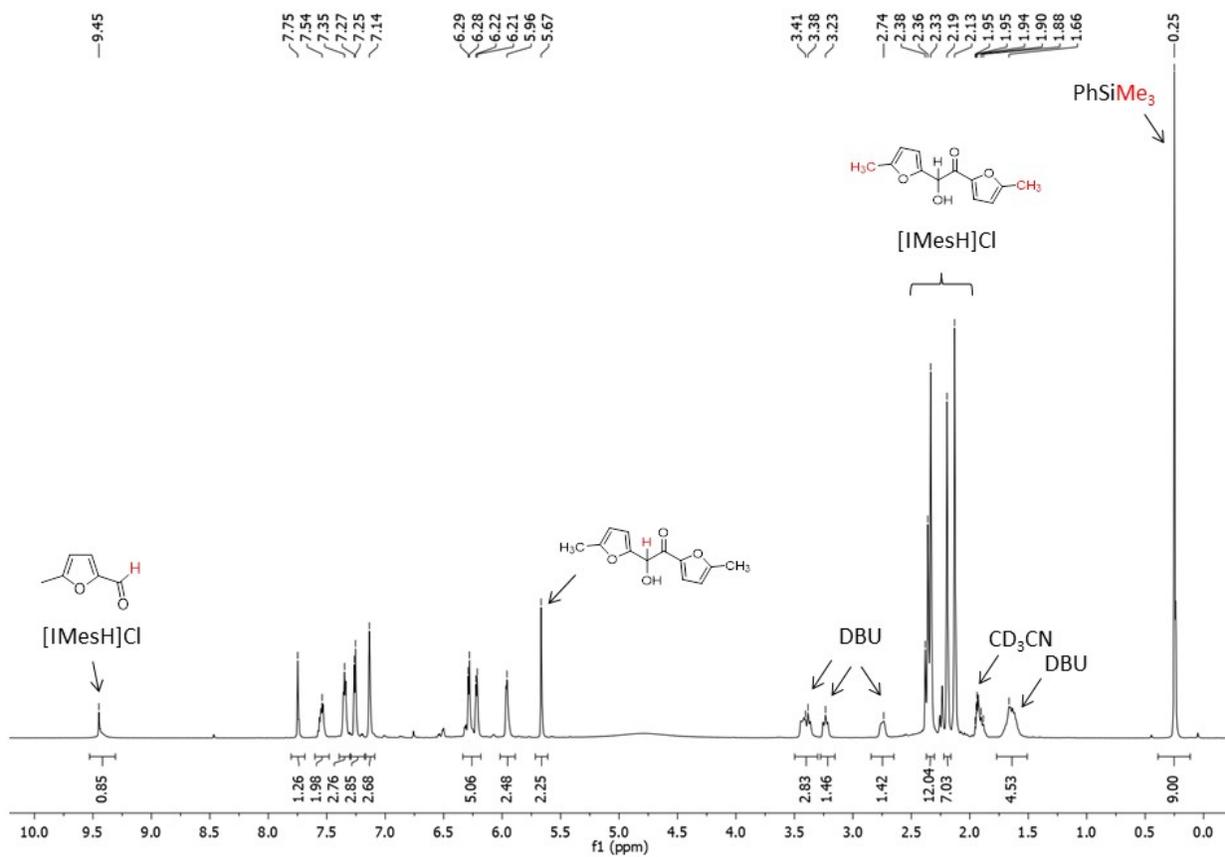


Figure S3. ^1H NMR spectra of the reaction mixture (conditions from entry 7, Table S1).

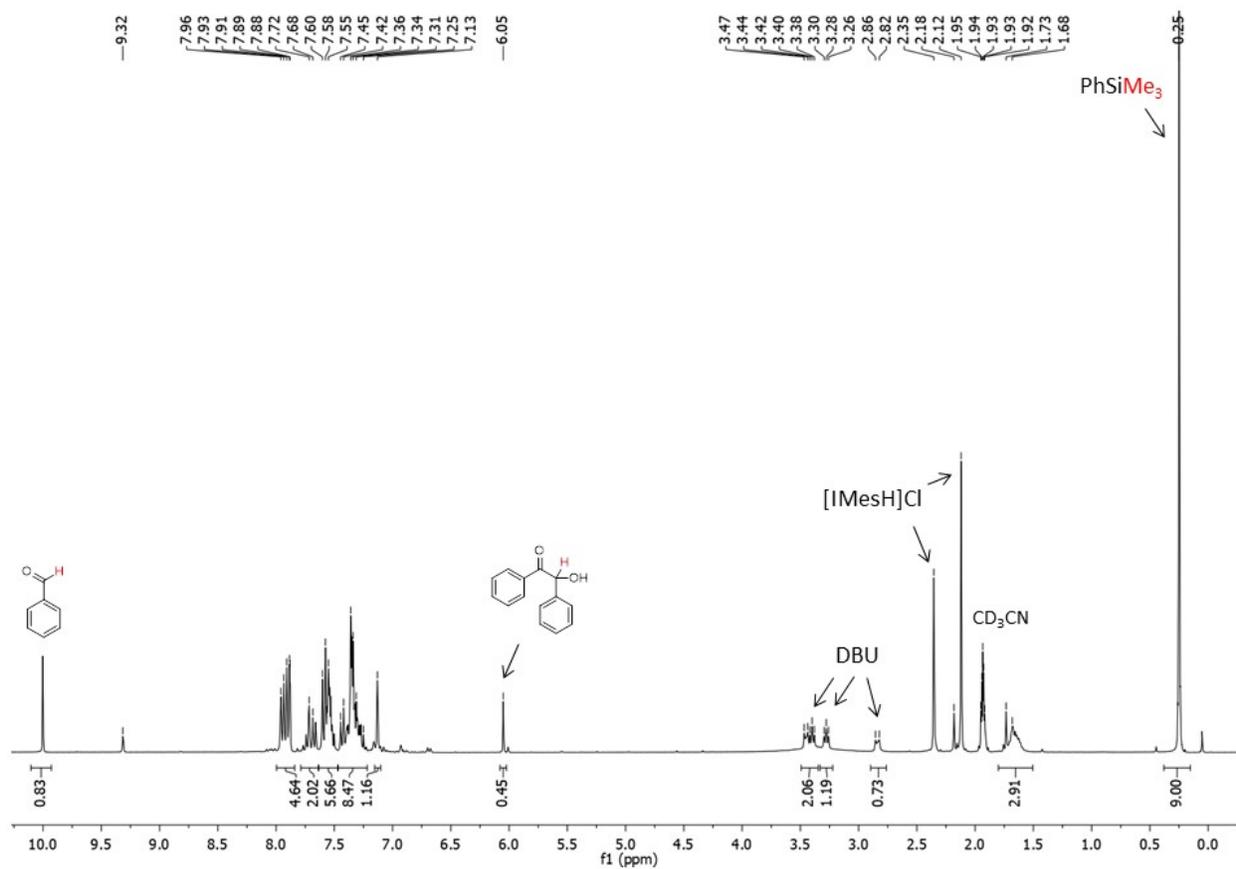


Figure S4. ^1H NMR spectra of the reaction mixture (conditions from entry 9, Table S1).

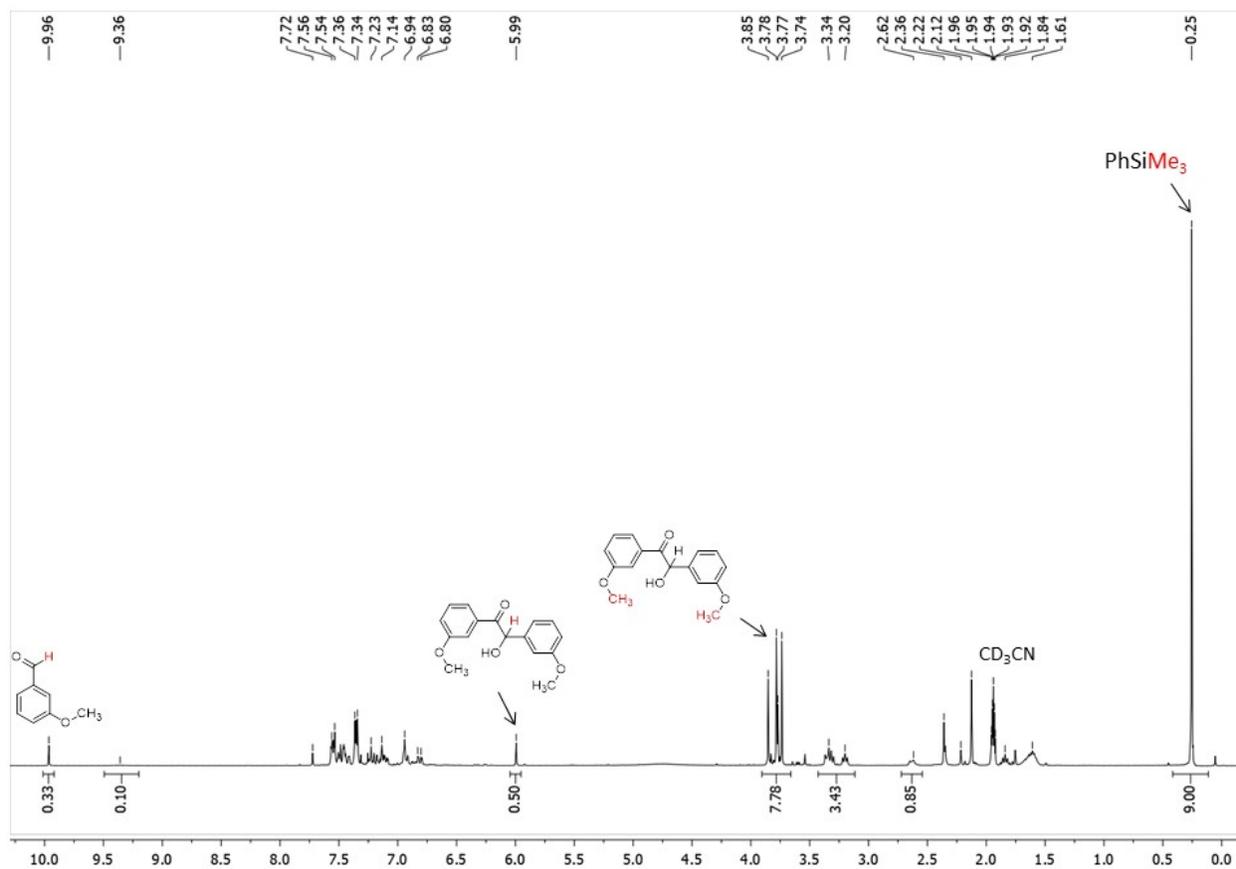


Figure S5. ^1H NMR spectra of the reaction mixture (conditions from entry 12, Table S1).

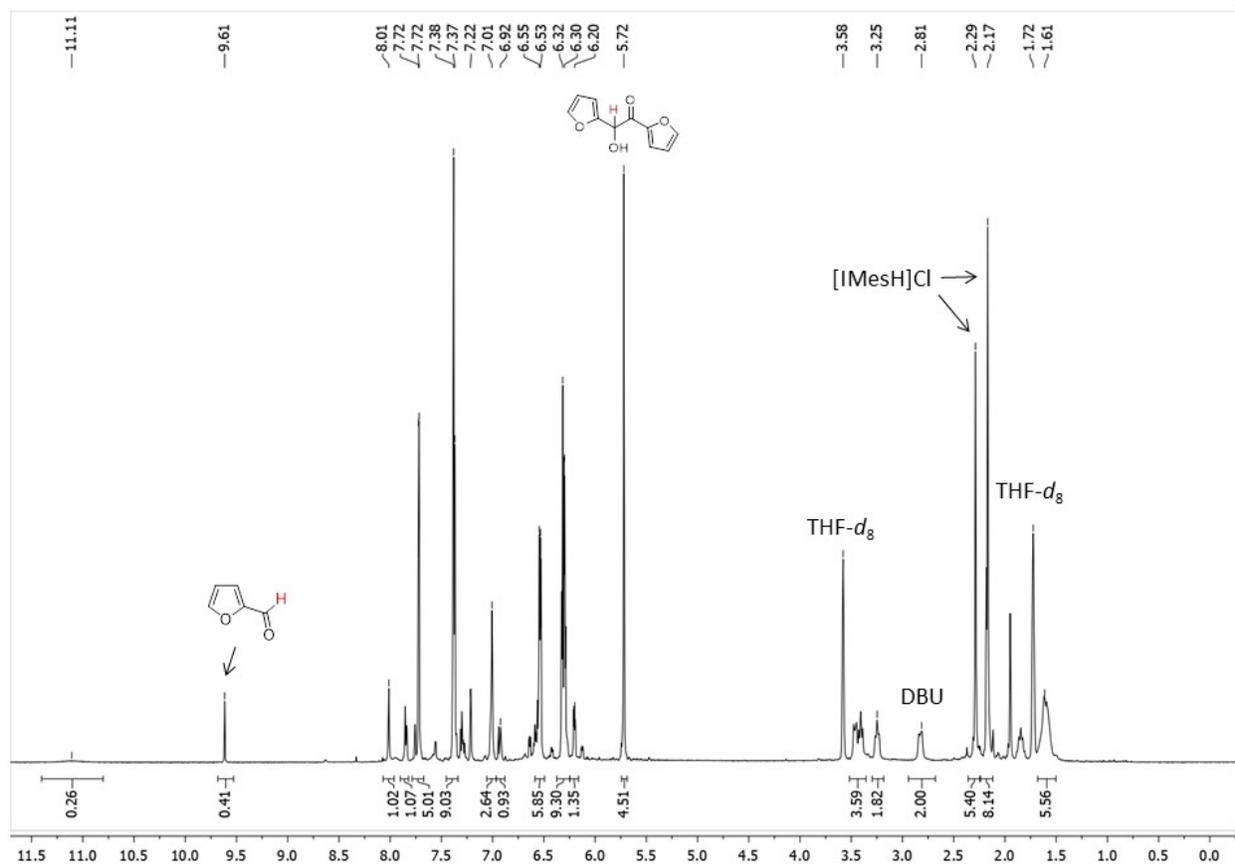


Figure S6. ^1H NMR spectra of the reaction mixture (conditions from entry 4, Table S2).

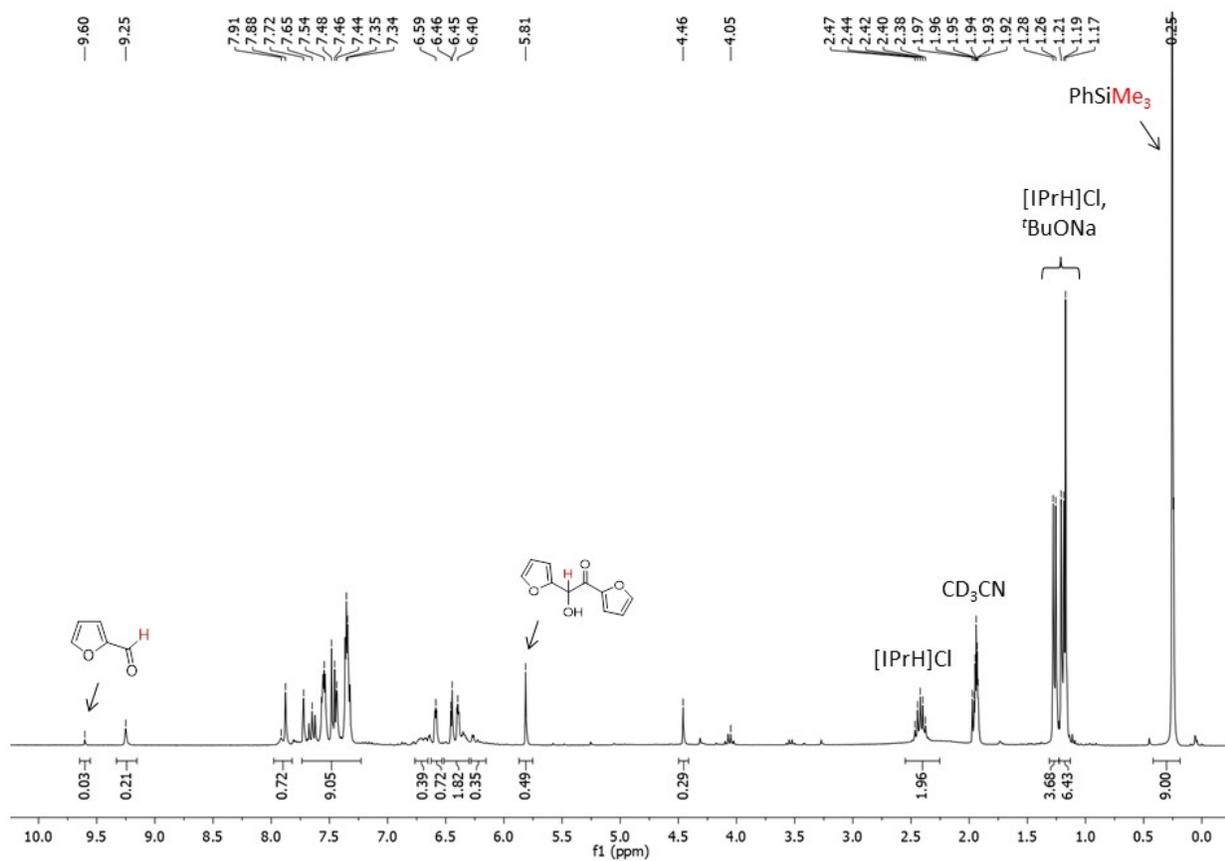


Figure S7. ^1H NMR spectra of the reaction mixture (conditions from entry 8, Table S2).

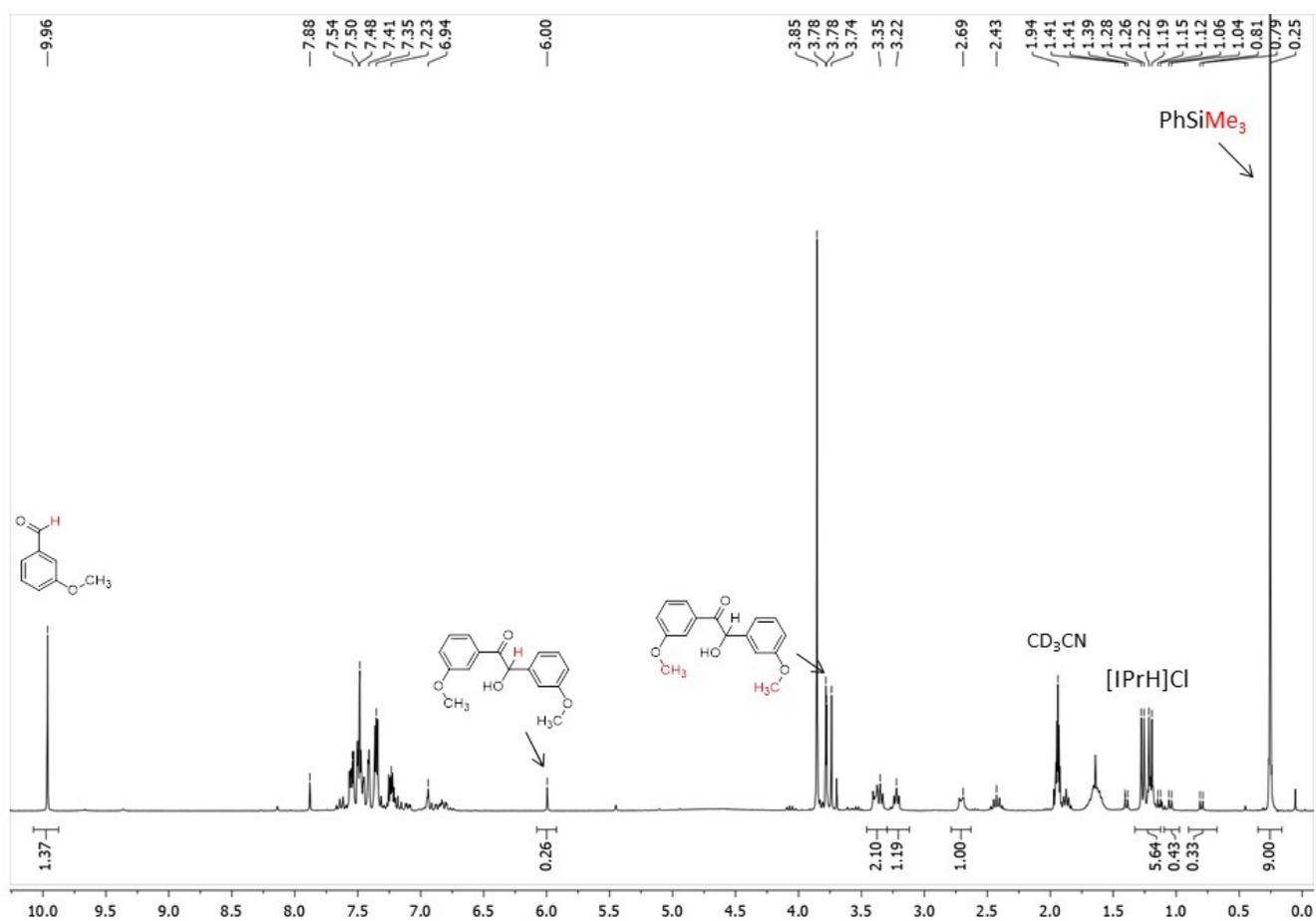
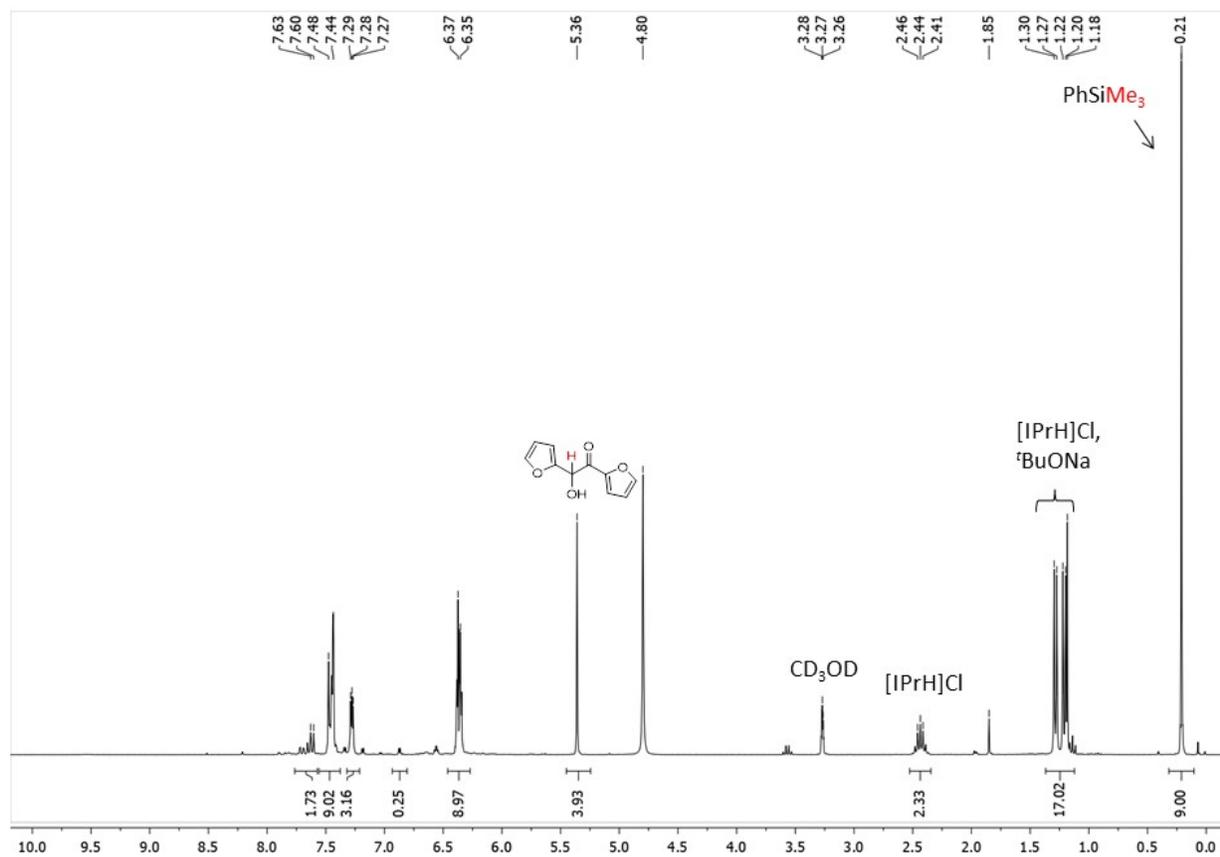


Figure S8. ^1H NMR spectra of the reaction mixture (conditions from entry 14, Table S2).

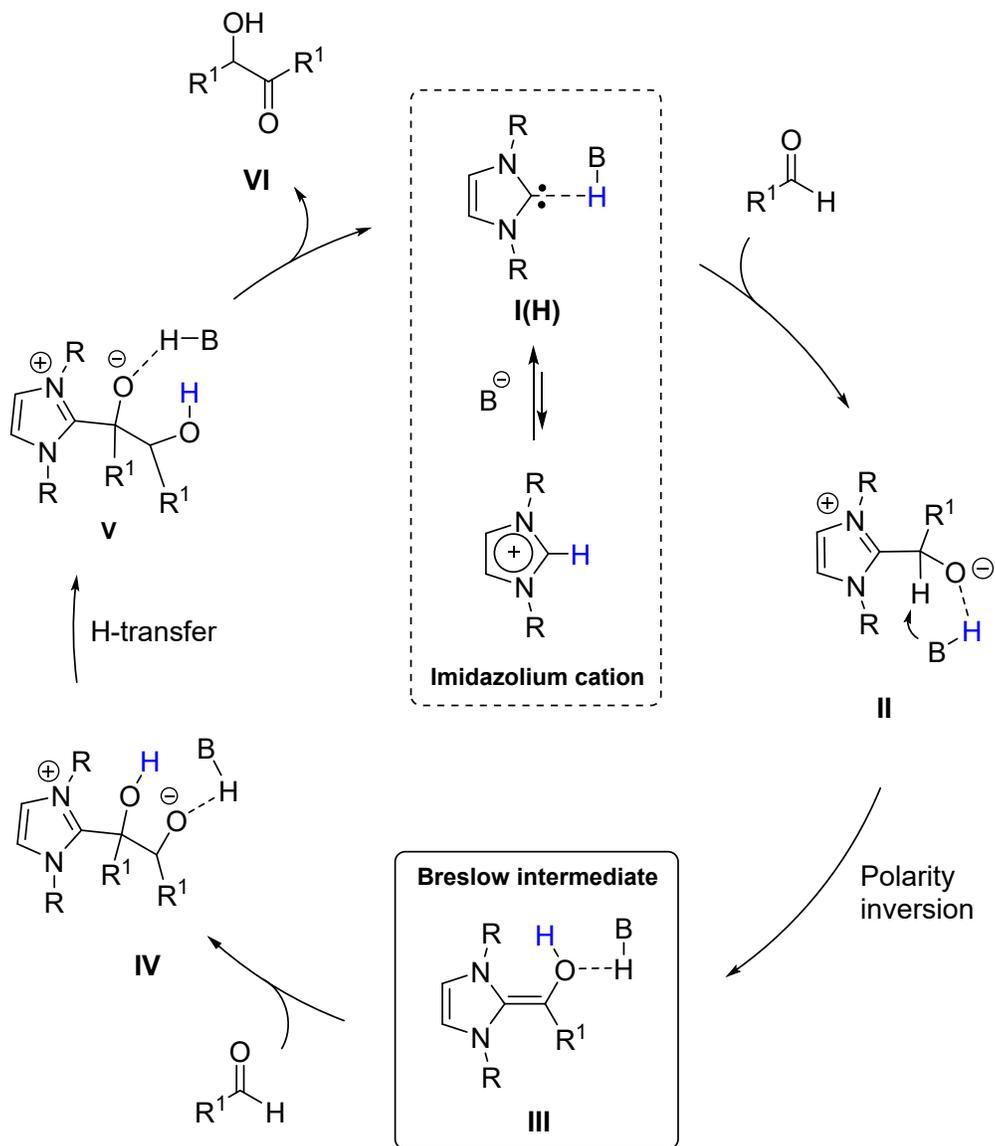


2. Computational details.

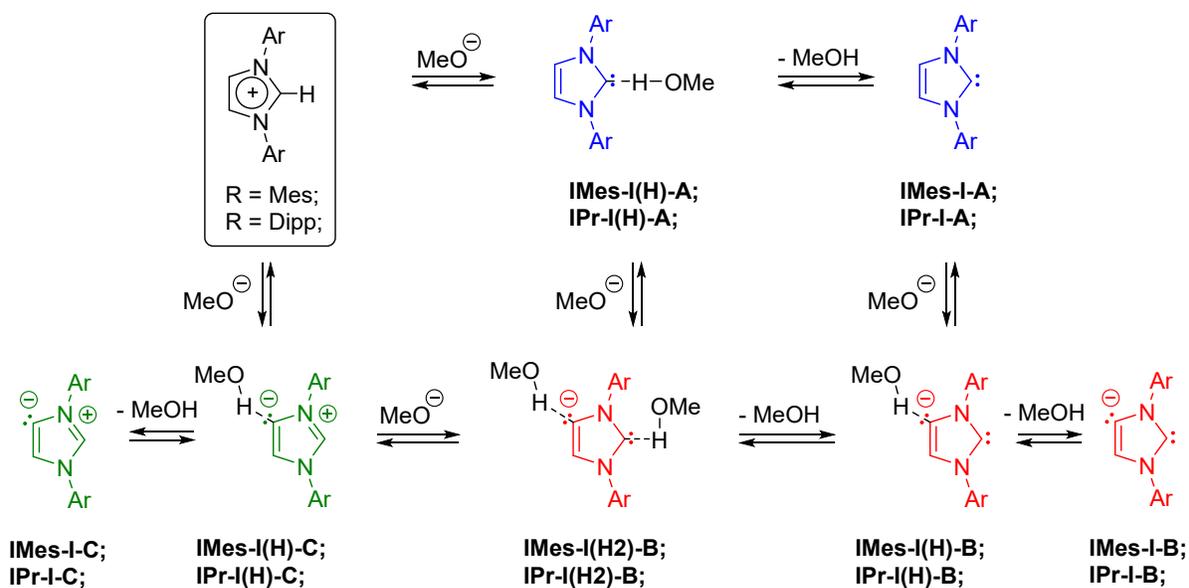
The reaction energy profiles of the benzoin condensation of furfural *via* paths A, B, and C (Schemes S3–S5) were calculated using the ORCA v.4.2.1 software^[1] at the PBE0/Def2TZVP level^[2] in the frame of the CPCM solvation model^[3] with MeOH parameters. For acceleration, the RIJCOSX approximation^[4] with the Def2/j fitting^[5] basis set was used. Frequencies and eigenvectors of normal modes were calculated in harmonic approximation for all the reaction participants; virtual modes were absent for the intermediates, whereas one virtual mode was found for the transition states. The optimized xyz-Cartesian coordinates are presented in Section 3. The calculated arbitrary energies for the reaction participants are provided in Table S3 (R = Mes) and Table S4 (R = Dipp). The orbital-weighted Fukui^[6] indices at the same level for the intermediates **IMes-III-A**, **IMes-III-B**, and **IMes-III-C** (Tables S7–S9) were calculated using the MultiWFN software v.3.7.^[7]

References:

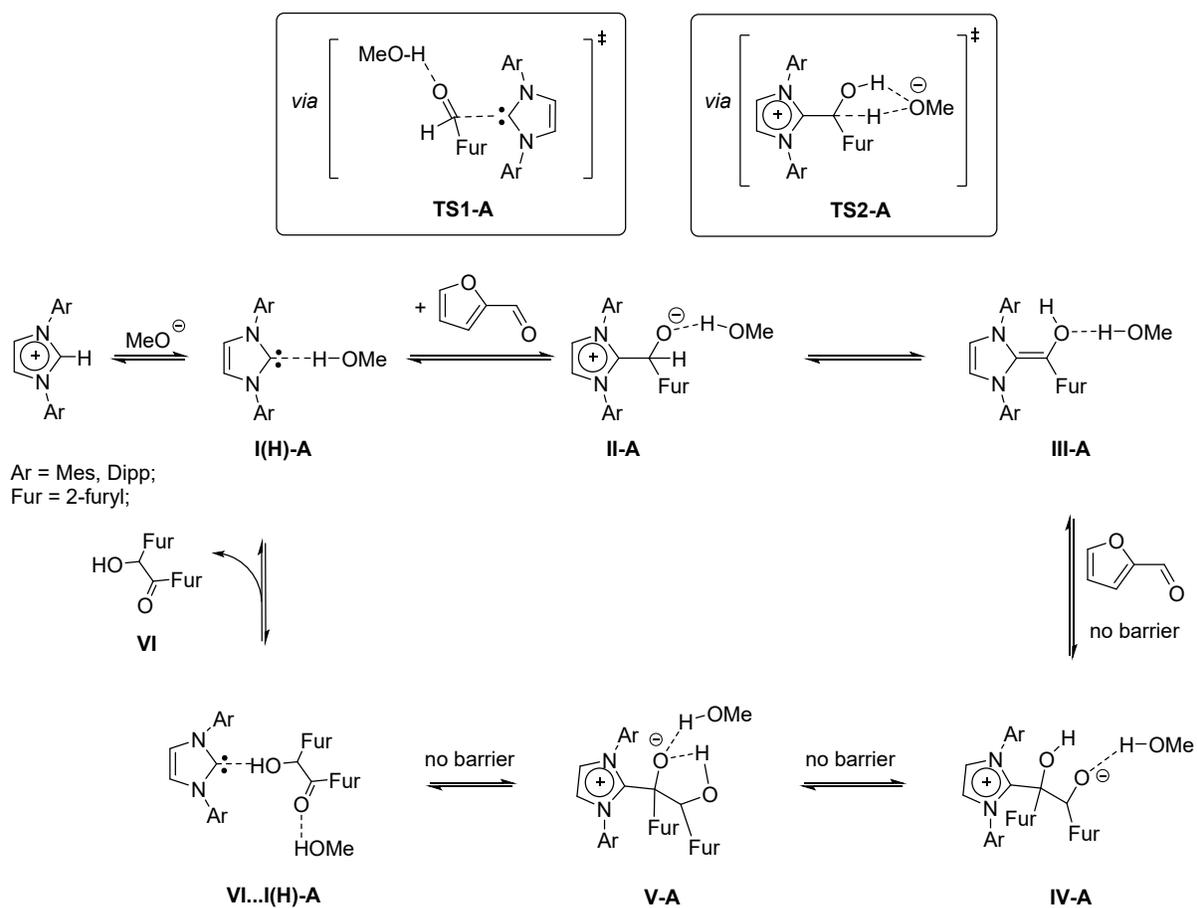
- [1](a) F. Neese, The ORCA program system. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2012**, 2, 73–78. (b) F. Neese, Software update: The ORCA program system, version 4.0. *Wiley Interdiscip. Rev. Comput. Mol. Sci.* **2018**, 8, e1327.
- [2](a) C. Adamo, V. Barone, *J. Chem. Phys.* **1999**, 110, 6158–6169. (b) F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, 7, 3297–3305.
- [3](a) A. Klamt, G. J. Schuurmann, *Chem. Soc., Perkin Trans.* **1993**, 2, 799. (b) J. Andzelm, C. Kölmel, A. J. Klamt, *Chem. Phys.* **1995**, 103, 9312–9320. (c) V. Barone, M. Cossi, *J. Phys. Chem. A* **1998**, 102, 1995–2001. (d) M. Cossi, N. Rega, G. Scalmani, V. Barone, *J. Comput. Chem.* **2003**, 24, 669–681.
- [4](a) F. Neese, *J. Comput. Chem.* **2003**, 24, 1740–1747. (b) F. Neese, F. Wennmohs, A. Hansen, U. Becker, *Chem. Phys.* **2009**, 356, 98–109. (c) A. K. Dutta, F. Neese, R. Izsak, *J. Chem. Phys.* **2016**, 144, 034102.
- [5] F. Weigend, *Phys. Chem. Chem. Phys.* **2006**, 8, 1057–1065.
- [6] R. Pino-Rios, D. Inostroza, G. Cárdenas-Jirón, W. Tiznado, *J. Phys. Chem. A*, **2019**, 123, 10556–10562.
- [7] Multiwfn Program, <http://sobereva.com/multiwfn/>



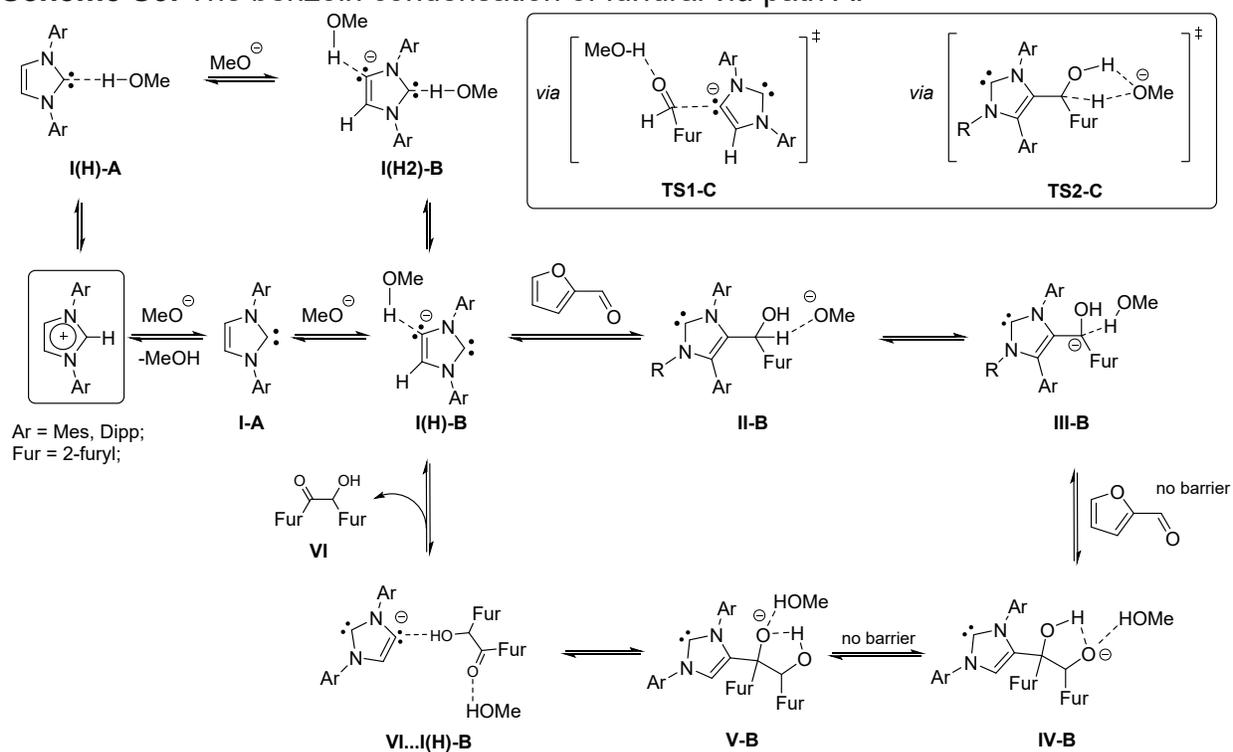
Scheme S1. Classical mechanism of the imidazolylidene-catalyzed benzoin condensation with involvement of the C2 carbene. B = base. R, R^1 = alkyl or aryl.



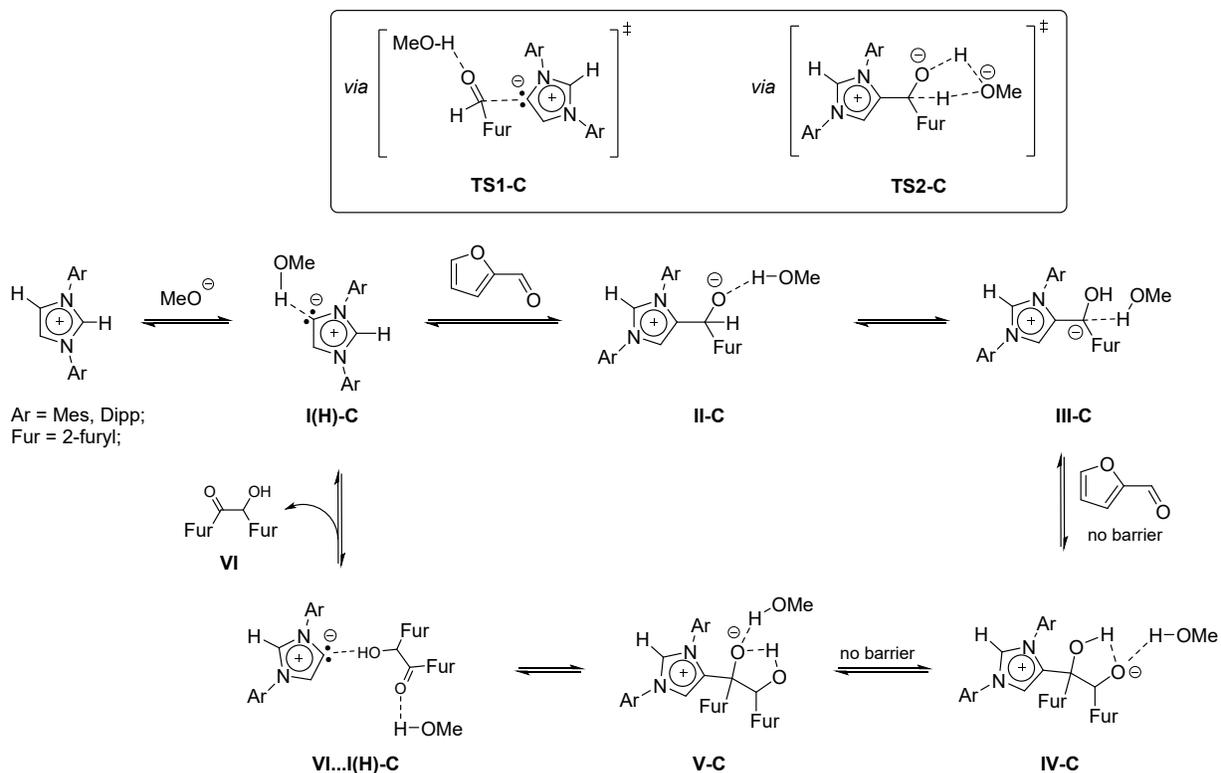
Scheme S2. Generation of the different imidazolium-derived carbenes.



Scheme S3. The benzoin condensation of furfural *via* path A.



Scheme S4. The benzoin condensation of furfural *via* path B.



Scheme S5. The benzoin condensation of furfural *via* path C.

Table S3. Arbitrary energy values for the benzoin condensation of furfural mediated by the [IMesH]⁺-derived catalytically active intermediates.

Reaction participant	ΔE_{tot} , kcal/mol	ΔH°_{298} , kcal/mol	ΔG°_{298} , kcal/mol
[IMesH]⁺	0.0	0.0	0.0
IMes-I(H)-A	-19.5	-19.1	-24.5
IMes-I-A	-14.0	-12.1	-31.8
IMes-TS1-A	-13.4	-12.2	-5.4
IMes-II-A	-28.5	-28.7	-18.1
IMes-TS2-A	-10.6	-9.6	-1.9
IMes-III-A	-24.5	-22.6	-17.0
IMes-IV-A	-24.2	-24.4	0.9
IMes-V-A	-27.6	-27.4	-2.9
VI...IMes-I(H)-A	-31.1	-30.3	-8.4
VI + IMes-I(H)-A	-26.5	-27.0	-17.6
IMes-I(H2)-B	-17.9	-17.1	-27.4
IMes-I(H)-B	-9.7	-7.9	-31.9
IMes-I-B	-1.6	1.3	-36.6
IMes-TS1-B	-0.2	1.1	-8.2
IMes-II-B	-37.8	-36.3	-45.2
IMes-TS2-B	-16.8	-15.9	-23.1
IMes-III-B	-17.6	-15.3	-26.0
IMes-IV-B	-45.6	-44.3	-38.2
IMes-V-B	-44.0	-43.1	-36.1
VI...IMes-I(H)-B	-34	-32.8	-27.0
VI + IMes-I(H)-B	-16.7	-15.8	-25.0
IMes-I(H)-C	-9.3	-9.0	-14.3
IMes-I-C	-2.3	0.2	-21.1
IMes-TS1-C	-2.7	-2.8	7.0
IMes-II-C	-28.7	-28.2	-19.6
IMes-TS2-C	-9.0	-8.9	0.8
IMes-III-C	-15.2	-13.8	-6.7
IMes-IV-C	-34.4	-34.4	-9.9
IMes-V-C	-34.2	-34.5	-9.6
VI...IMes-I(H)-C	-24.7	-25.0	-0.4
VI + IMes-I(H)-C	-16.3	-16.9	-7.4
Furfural	0.0	0.0	0.0
VI	-7.0	-7.9	6.9

Table S4. Arbitrary energy values for the benzoin condensation of furfural, benzaldehyde and isobutyraldehyde mediated by the [IPrH]⁺-derived catalytically active intermediates.

Reaction participant	ΔE_{tot} , kcal/mol	ΔH°_{298} , kcal/mol	ΔG°_{298} , kcal/mol
[IPrH] ⁺	0.0	0.0	0.0
IPr-I(H)-A	-21.9	-21.8	-26.1
IPr-I-A	-15.0	-14.1	-31.7
IPr-TS1-A	-12.3	-11.9	-2.6
IPr-II-A	-29.9	-29.2	-20.4
IPr-TS2-A	-9.1	-8.8	1.2
IPr-III-A	-23.7	-23.1	-13.5
IPr-IV-A	-23.8	-23.8	1.3
IPr-V-A	-25.3	-25.7	0.1
VI...IPr-I(H)-A	-34.4	-32.8	-12.5
VI + IPr-I(H)-A	-28.9	-29.7	-19.2
IPr-TS1 ^{Ph} -A	-11.0	-10.8	-0.8
IPr-II ^{Ph} -A	-28.6	-28.1	-18.3
IPr-TS2 ^{Ph} -A	-6.6	-6.3	4.0
IPr-III ^{Ph} -A	-20.8	-19.8	-10.9
IPr-TS1 ^{iPr} -A	-13.1	-12.4	-4.4
IPr-II ^{iPr} -A	-29.1	-28.9	-19.4
IPr-TS2 ^{iPr} -A	-6.8	-7.0	3.7
IPr-III ^{iPr} -A	-18.0	-17.6	-8.4
IPr-I(H2)-B	-22.6	-21.0	-33.2
IPr-I(H)-B	-14.1	-12.1	-36.8
IPr-I-B	0.7	1.5	-31.2
IPr-TS1-B	-18.8	-17.3	-25.8
IPr-II-B	-41.7	-40.2	-48.9
IPr-TS2-B	-16.2	-25.7	-32.0
IPr-III-B	-47.7	-46.7	-40.1
IPr-IV-B	-46.9	-45.7	-39.1
IPr-V-B	-39.9	-37.4	-35.4
VI...IPr-I(H)-B	-27.3	-26.3	-35.9
VI + IPr-I(H)-B	-21.1	-20.0	-29.0
IPr-TS1 ^{Ph} -B	-14.7	-13.0	-22.0
IPr-II ^{Ph} -B	-40.3	-38.8	-47.2
IPr-TS2 ^{Ph} -B	-16.3	-14.8	-22.9
IPr-III ^{Ph} -B	-18.8	-16.5	-26.6

IPr-TS1^{iPr}-B	-12.7	-11.8	-19.8
IPr-II^{iPr}-B	-40.9	-40.1	-47.7
IPr-TS2^{iPr}-B	-7.0	-5.7	-13.9
IPr-III^{iPr}-B	-1.3	0.5	-9.1

Table S5. Calculated energies (kcal mol⁻¹) for the deprotonation of *N*-alkyl and *N*-aryl substituted imidazolium cations and C2 carbenes.

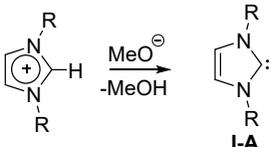
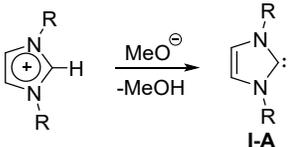
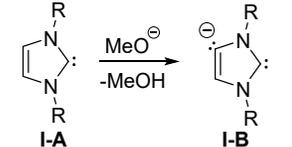
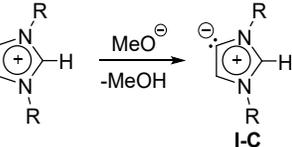
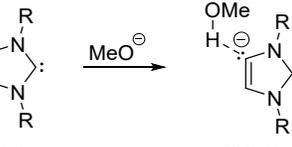
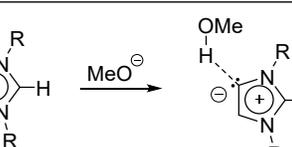
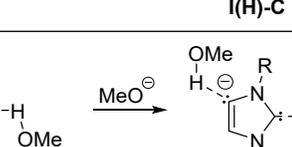
R=	Me		ⁱ Pr		^t Bu		Mes		Dipp	
Reaction	ΔH_{298}°	ΔG_{298}°	ΔH_{298}°	ΔG_{298}°	ΔH_{298}°	ΔG_{298}°	ΔH_{298}°	ΔG_{298}°	ΔH_{298}°	ΔG_{298}°
	-11.5	-28.9	-9.4	-28.3	-8.6	-26.9	-12.1	-31.8	-14.1	-31.7
	16.2	-1.4	17.1	-0.4	18.3	1.8	13.5	-4.8	15.6	0.5

Table S6. Calculated energies (kcal mol⁻¹) for the deprotonation of *N*-aryl substituted imidazolium cations and various carbenes.

Entry	Reaction	R = Mes		R = Dipp	
		ΔH°_{298}	ΔG°_{298}	ΔH°_{298}	ΔG°_{298}
1		-12.1	-31.8	-14.1	-31.7
2		13.5	-4.8	15.6	0.5
3		0.2	-21.1	-2.2	-19.8
4		-19.1	-24.5	-21.8	-26.1
5		4.3	-0.1	2.0	-5.1
6		-9.0	-14.3	-8.3	-15.4
7		2.0	-3.0	0.8	-7.1

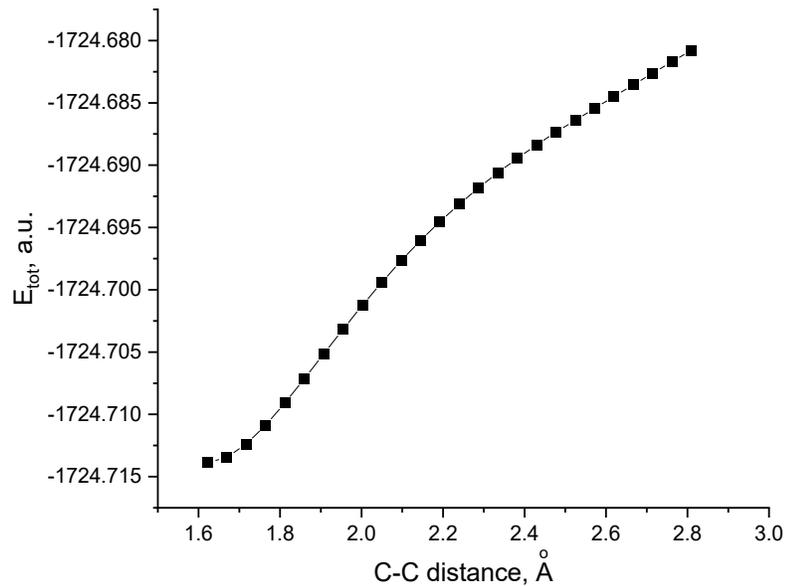


Figure S9. PES scan for the addition of second molecule of furfural (stage from **IMes-III-B** to **IMes-VI-B**).

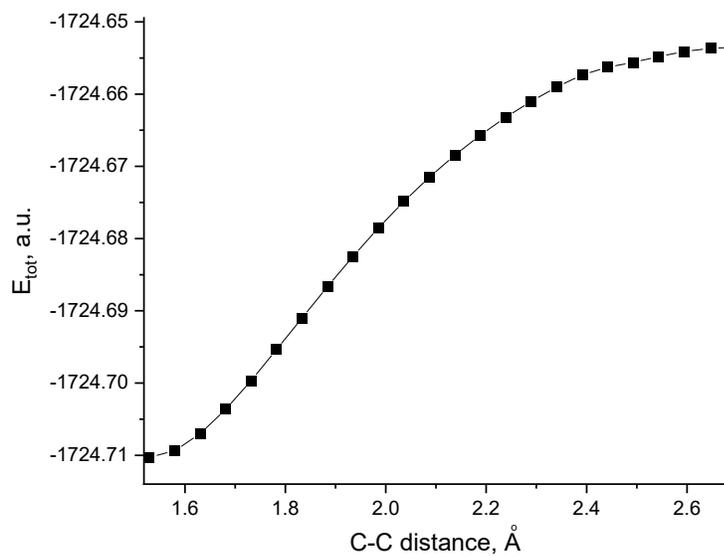


Figure S10. PES scan for the elimination of NHC (stage from **IMes-V-B** to **VI....IMes-I(H)-B**).

Table S7. Fukui indices (\bar{e}) for **IMes-III-A**.

Atom	f_w^+	f_w^-	$f_w^0 = f_w^+ + f_w^-$	$f_w^{DD} = f_w^+ - f_w^-$
1(C)	0.04798	0.06187	0.05493	-0.01389
2(C)	0.00848	0.06086	0.03467	-0.05238
3(H)	0.00161	0.00623	0.00392	-0.00462
4(C)	0.01090	0.06279	0.03684	-0.05189
5(H)	0.00220	0.00650	0.00435	-0.00430
6(N)	0.02259	0.08053	0.05156	-0.05794
7(N)	0.02386	0.07857	0.05121	-0.05471
8(C)	0.06799	0.00841	0.03820	0.05959
9(C)	0.02750	0.00378	0.01564	0.02372
10(C)	0.05421	0.00425	0.02923	0.04996
11(C)	0.04597	0.00084	0.02340	0.04512
12(C)	0.02622	0.00104	0.01363	0.02517
13(C)	0.07604	0.00102	0.03853	0.07501
14(H)	0.00743	0.00021	0.00382	0.00722
15(H)	0.00283	0.00033	0.00158	0.00250
16(C)	0.06335	0.00842	0.03588	0.05493
17(C)	0.03913	0.00320	0.02117	0.03593
18(C)	0.02960	0.00404	0.01682	0.02556
19(C)	0.02661	0.00062	0.01362	0.02599
20(C)	0.03392	0.00095	0.01744	0.03297
21(C)	0.07023	0.00046	0.03535	0.06977
22(H)	0.00321	0.00020	0.00170	0.00301
23(H)	0.00518	0.00032	0.00275	0.00486
24(C)	0.00625	0.00253	0.00439	0.00371
25(H)	0.00302	0.00372	0.00337	-0.00070
26(H)	0.00242	0.00121	0.00181	0.00121
27(H)	0.00141	0.00028	0.00085	0.00113
28(C)	0.00765	0.00087	0.00426	0.00679
29(H)	0.00365	0.00092	0.00228	0.00273
30(H)	0.00307	0.00024	0.00165	0.00282
31(H)	0.00122	0.00004	0.00063	0.00119
32(C)	0.00559	0.00102	0.00331	0.00457
33(H)	0.00268	0.00090	0.00179	0.00177
34(H)	0.00166	0.00051	0.00109	0.00115
35(H)	0.00163	0.00005	0.00084	0.00158
36(C)	0.01032	0.00266	0.00649	0.00765
37(H)	0.00512	0.00335	0.00424	0.00177
38(H)	0.00400	0.00107	0.00253	0.00292
39(H)	0.00135	0.00039	0.00087	0.00096
40(C)	0.01324	0.00019	0.00672	0.01305

41(H)	0.00981	0.00015	0.00498	0.00966
42(H)	0.00271	0.00003	0.00137	0.00268
43(H)	0.00327	0.00005	0.00166	0.00322
44(C)	0.01210	0.00008	0.00609	0.01203
45(H)	0.00863	0.00004	0.00433	0.00859
46(H)	0.00313	0.00001	0.00157	0.00312
47(H)	0.00243	0.00003	0.00123	0.00240
48(C)	0.02350	0.21413	0.11881	-0.19064
49(O)	0.00765	0.04686	0.02725	-0.03921
50(H)	0.00146	0.00226	0.00186	-0.00081
51(C)	0.03155	0.04675	0.03915	-0.01520
52(C)	0.02520	0.09747	0.06134	-0.07227
53(O)	0.02163	0.02046	0.02104	0.00117
54(C)	0.01328	0.03292	0.02310	-0.01964
55(H)	0.00358	0.01016	0.00687	-0.00659
56(C)	0.03105	0.08583	0.05844	-0.05478
57(H)	0.00148	0.00267	0.00207	-0.00119
58(H)	0.00684	0.00983	0.00833	-0.00299
59(O)	0.00105	0.00137	0.00121	-0.00032
60(C)	0.00051	0.00035	0.00043	0.00015
61(H)	0.00007	0.00004	0.00005	0.00003
62(H)	0.00052	0.00053	0.00053	-0.00001
63(H)	0.00023	0.00009	0.00016	0.00014
64(H)	0.00348	0.01234	0.00791	-0.00886

Table S8. Fukui indices (\bar{e}) for **IMes-III-B**.

Atom	f_w^+	f_w^-	$f_w^0 = f_w^{++} + f_w^{--}$	$f_w^{DD} = f_w^{+-} - f_w^{-+}$
1(C)	0.04733	0.06160	0.05446	-0.01427
2(C)	0.01633	0.12976	0.07305	-0.11343
3(H)	0.00232	0.01518	0.00875	-0.01286
4(C)	0.01562	0.05709	0.03635	-0.04147
5(H)	0.00088	0.01121	0.00605	-0.01033
6(N)	0.03402	0.02860	0.03131	0.00541
7(N)	0.03003	0.04183	0.03593	-0.01180
8(C)	0.10704	0.00415	0.05559	0.10289
9(C)	0.06345	0.00180	0.03263	0.06166
10(C)	0.05493	0.00194	0.02844	0.05299
11(C)	0.04765	0.00039	0.02402	0.04726
12(C)	0.05212	0.00046	0.02629	0.05166
13(C)	0.12132	0.00042	0.06087	0.12090

14(H)	0.00599	0.00010	0.00305	0.00589
15(H)	0.00724	0.00013	0.00368	0.00711
16(C)	0.04931	0.00344	0.02638	0.04587
17(C)	0.02422	0.00109	0.01265	0.02313
18(C)	0.03513	0.00118	0.01816	0.03395
19(C)	0.02735	0.00027	0.01381	0.02708
20(C)	0.02014	0.00029	0.01021	0.01985
21(C)	0.05161	0.00006	0.02583	0.05155
22(H)	0.00420	0.00006	0.00213	0.00415
23(H)	0.00221	0.00006	0.00113	0.00215
24(C)	0.00641	0.00189	0.00415	0.00452
25(H)	0.00361	0.00091	0.00226	0.00270
26(H)	0.00267	0.00265	0.00266	0.00001
27(H)	0.00123	0.00014	0.00068	0.00109
28(C)	0.00577	0.00192	0.00384	0.00385
29(H)	0.00158	0.00263	0.00210	-0.00105
30(H)	0.00514	0.00088	0.00301	0.00426
31(H)	0.00127	0.00013	0.00070	0.00115
32(C)	0.01172	0.00074	0.00623	0.01098
33(H)	0.00609	0.00163	0.00386	0.00446
34(H)	0.00386	0.00042	0.00214	0.00345
35(H)	0.00200	0.00003	0.00101	0.00197
36(C)	0.01273	0.00089	0.00681	0.01184
37(H)	0.00915	0.00103	0.00509	0.00811
38(H)	0.00385	0.00123	0.00254	0.00262
39(H)	0.00264	0.00006	0.00135	0.00258
40(C)	0.02034	0.00007	0.01021	0.02027
41(H)	0.01385	0.00003	0.00694	0.01382
42(H)	0.00345	0.00001	0.00173	0.00344
43(H)	0.00602	0.00003	0.00302	0.00599
44(C)	0.00883	0.00001	0.00442	0.00881
45(H)	0.00587	0.00000	0.00294	0.00587
46(H)	0.00139	0.00000	0.00069	0.00138
47(H)	0.00290	0.00000	0.00145	0.00290
48(H)	0.00942	0.00757	0.00849	0.00184
49(O)	0.00208	0.00204	0.00206	0.00004
50(C)	0.00072	0.00028	0.00050	0.00044
51(H)	0.00023	0.00008	0.00016	0.00015
52(H)	0.00017	0.00014	0.00015	0.00003
53(H)	0.00051	0.00010	0.00030	0.00041
54(C)	0.00498	0.22751	0.11624	-0.22252
55(O)	0.00292	0.04624	0.02458	-0.04332
56(C)	0.00285	0.04421	0.02353	-0.04136

57(C)	0.00200	0.11567	0.05884	-0.11366
58(O)	0.00136	0.02363	0.01249	-0.02227
59(C)	0.00084	0.03255	0.01670	-0.03171
60(H)	0.00032	0.01362	0.00697	-0.01330
61(C)	0.00201	0.09395	0.04798	-0.09195
62(H)	0.00009	0.00242	0.00125	-0.00232
63(H)	0.00032	0.01133	0.00583	-0.01102
64(H)	0.00521	0.00018	0.00270	0.00503

Table S9. Fukui indexes (\bar{e}) for **IMes-III-C**.

Atom	f_w^+	f_w^-	$f_w^0 = f_w^+ + f_w^-$	$f_w^{DD} = f_w^+ - f_w^-$
1(C)	0.00118	0.12125	0.06122	-0.12008
2(C)	0.00058	0.04740	0.02399	-0.04682
3(N)	0.00185	0.03472	0.01828	-0.03287
4(C)	0.00218	0.03859	0.02039	-0.03641
5(N)	0.00084	0.01554	0.00819	-0.01470
6(H)	0.00022	0.01362	0.00692	-0.01340
7(O)	0.00003	0.02418	0.01210	-0.02415
8(C)	0.00017	0.23179	0.11598	-0.23162
9(O)	0.00008	0.04531	0.02269	-0.04523
10(H)	0.00004	0.01112	0.00558	-0.01108
11(C)	0.00002	0.00361	0.00181	-0.00359
12(H)	0.00000	0.00172	0.00086	-0.00172
13(H)	0.00000	0.00197	0.00098	-0.00196
14(H)	0.00003	0.00052	0.00027	-0.00049
15(H)	0.00003	0.02626	0.01314	-0.02623
16(C)	0.00010	0.04542	0.02276	-0.04532
17(C)	0.00007	0.12211	0.06109	-0.12204
18(O)	0.00010	0.02552	0.01281	-0.02542
19(C)	0.00003	0.03406	0.01704	-0.03403
20(H)	0.00001	0.01441	0.00721	-0.01440
21(C)	0.00008	0.10013	0.05010	-0.10004
22(H)	0.00000	0.00256	0.00128	-0.00256
23(H)	0.00002	0.01228	0.00615	-0.01227
24(C)	0.01161	0.00420	0.00791	0.00741
25(C)	0.00554	0.00201	0.00377	0.00353
26(C)	0.00708	0.00199	0.00454	0.00509
27(C)	0.00658	0.00040	0.00349	0.00618
28(C)	0.00528	0.00042	0.00285	0.00485
29(C)	0.01279	0.00093	0.00686	0.01185
30(H)	0.00099	0.00007	0.00053	0.00092

31(H)	0.00068	0.00011	0.00039	0.00057
32(C)	0.00222	0.00145	0.00184	0.00076
33(C)	0.00077	0.00063	0.00070	0.00014
34(C)	0.00211	0.00046	0.00129	0.00165
35(C)	0.00186	0.00016	0.00101	0.00171
36(C)	0.00079	0.00011	0.00045	0.00068
37(C)	0.00231	0.00004	0.00118	0.00227
38(H)	0.00034	0.00005	0.00019	0.00029
39(H)	0.00007	0.00002	0.00005	0.00004
40(C)	0.00019	0.00045	0.00032	-0.00026
41(H)	0.00012	0.00032	0.00022	-0.00021
42(H)	0.00006	0.00085	0.00045	-0.00080
43(H)	0.00006	0.00002	0.00004	0.00004
44(C)	0.00041	0.00051	0.00046	-0.00010
45(H)	0.00022	0.00054	0.00038	-0.00033
46(H)	0.00019	0.00079	0.00049	-0.00060
47(H)	0.00004	0.00005	0.00005	-0.00001
48(C)	0.00044	0.00001	0.00023	0.00044
49(H)	0.00024	0.00000	0.00012	0.00024
50(H)	0.00027	0.00000	0.00014	0.00026
51(H)	0.00004	0.00000	0.00002	0.00004
52(C)	0.00113	0.00151	0.00132	-0.00038
53(H)	0.00037	0.00120	0.00079	-0.00083
54(H)	0.00060	0.00101	0.00081	-0.00042
55(H)	0.00027	0.00019	0.00023	0.00007
56(C)	0.00141	0.00189	0.00165	-0.00048
57(H)	0.00050	0.00089	0.00070	-0.00039
58(H)	0.00080	0.00206	0.00143	-0.00126
59(H)	0.00026	0.00023	0.00025	0.00002
60(C)	0.00225	0.00015	0.00120	0.00210
61(H)	0.00159	0.00009	0.00084	0.00151
62(H)	0.00047	0.00004	0.00025	0.00043
63(H)	0.00059	0.00003	0.00031	0.00056

3. Optimized xyz-Cartesian coordinates.

[IMesH]⁺ Etot = -923.903511504590 a.u.

C	0.000003000	-0.000153000	-0.148940000
C	0.677701000	0.001787000	1.936168000
H	1.387746000	0.002536000	2.745610000
C	-0.677702000	0.001793000	1.936166000
H	-1.387749000	0.002495000	2.745606000
N	1.082263000	0.000559000	0.622104000
N	-1.082260000	0.000573000	0.622101000
C	-2.445121000	0.000101000	0.154344000
C	-3.076416000	1.226441000	-0.049255000
C	-3.075332000	-1.226791000	-0.050074000
C	-4.395646000	1.194578000	-0.481075000
C	-4.394478000	-1.195892000	-0.481825000
C	-5.070707000	-0.000843000	-0.705164000
H	-4.911997000	2.134830000	-0.643518000
H	-4.909974000	-2.136533000	-0.644839000
C	2.445126000	0.000148000	0.154353000
C	3.076052000	-1.226576000	-0.048000000
C	3.075707000	1.226654000	-0.051308000
C	4.395304000	-1.195544000	-0.479849000
C	4.394835000	1.194924000	-0.483020000
C	5.070716000	-0.000561000	-0.705145000
H	4.911382000	-2.136112000	-0.641317000
H	4.910605000	2.135248000	-0.647004000
C	2.374462000	2.530124000	0.182784000
H	1.510709000	2.651478000	-0.477183000
H	2.013993000	2.621343000	1.210826000
H	3.049045000	3.363900000	-0.005902000
C	2.375341000	-2.529706000	0.189544000
H	2.015104000	-2.618449000	1.217882000
H	1.511499000	-2.653049000	-0.469933000
H	3.050197000	-3.363711000	0.002857000
C	-2.376089000	2.530016000	0.186972000
H	-2.016841000	2.620360000	1.215520000
H	-1.511630000	2.652467000	-0.471858000
H	-3.050877000	3.363652000	-0.001595000
C	-2.373713000	-2.529818000	0.185365000
H	-1.510439000	-2.651992000	-0.475079000
H	-2.012465000	-2.619506000	1.213266000
H	-3.048303000	-3.363967000	-0.001641000
C	-6.483916000	-0.001717000	-1.196458000
H	-6.507253000	-0.015634000	-2.290267000
H	-7.027071000	-0.880674000	-0.847369000

H	-7.020762000	0.889434000	-0.869514000
C	6.483929000	-0.000538000	-1.196425000
H	6.507294000	0.014621000	-2.290217000
H	7.027923000	0.877520000	-0.846356000
H	7.019917000	-0.892555000	-0.870461000
H	0.000004000	-0.001125000	-1.226745000

IMes-I-A

Etot = -923.406887250205 a.u.

C	-0.000003000	-0.000582000	-0.277228000
C	0.673950000	0.002333000	1.910466000
H	1.381805000	0.003381000	2.722671000
C	-0.673940000	0.002312000	1.910471000
H	-1.381788000	0.003328000	2.722683000
N	1.055655000	0.000563000	0.580087000
N	-1.055656000	0.000550000	0.580097000
C	-2.416842000	0.000090000	0.152611000
C	-3.066429000	1.217261000	-0.045278000
C	-3.065041000	-1.217645000	-0.047245000
C	-4.399184000	1.192043000	-0.438845000
C	-4.397686000	-1.193398000	-0.440786000
C	-5.081999000	-0.000866000	-0.641530000
H	-4.916031000	2.134442000	-0.594107000
H	-4.913403000	-2.136184000	-0.597548000
C	2.416844000	0.000109000	0.152614000
C	3.065976000	-1.217463000	-0.044215000
C	3.065502000	1.217441000	-0.048295000
C	4.398747000	-1.193065000	-0.437820000
C	4.398136000	1.192374000	-0.441782000
C	5.082008000	-0.000593000	-0.641511000
H	4.915258000	-2.135784000	-0.592242000
H	4.914189000	2.134839000	-0.599377000
C	2.341103000	2.514971000	0.134762000
H	1.487456000	2.577347000	-0.544870000
H	1.946726000	2.618262000	1.149038000
H	3.003893000	3.358211000	-0.061244000
C	2.342309000	-2.514784000	0.143186000
H	1.947872000	-2.614848000	1.157758000
H	1.488779000	-2.580007000	-0.536326000
H	3.005614000	-3.358304000	-0.049857000
C	-2.343203000	2.515010000	0.140908000
H	-1.949644000	2.616633000	1.155669000
H	-1.489124000	2.579493000	-0.537982000
H	-3.006537000	3.358106000	-0.053877000
C	-2.340209000	-2.514750000	0.137061000
H	-1.486952000	-2.577774000	-0.542999000

H	-1.945194000	-2.616573000	1.151236000
H	-3.002903000	-3.358415000	-0.057438000
C	-6.510012000	-0.001663000	-1.097889000
H	-6.569491000	-0.014930000	-2.190692000
H	-7.044840000	-0.880068000	-0.731942000
H	-7.038959000	0.888780000	-0.753345000
C	6.510027000	-0.000664000	-1.097849000
H	6.569539000	0.014006000	-2.190633000
H	7.045754000	0.876719000	-0.730748000
H	7.038051000	-0.892093000	-0.754458000

IMes-I(H)-A

Etot = -1039.061571616990 a.u.

C	-1.795898000	0.449182000	-0.210980000
C	-2.492429000	2.274637000	-1.375880000
H	-3.197762000	3.010479000	-1.723669000
C	-1.187017000	2.093176000	-1.660575000
N	-2.838160000	1.268097000	-0.493993000
N	-0.786712000	0.982905000	-0.940937000
C	0.543928000	0.462663000	-0.963766000
C	1.529372000	1.107374000	-0.213035000
C	0.823188000	-0.667823000	-1.728699000
C	2.821125000	0.602079000	-0.257770000
C	2.134285000	-1.135132000	-1.740092000
C	3.145138000	-0.515544000	-1.019687000
H	3.594030000	1.090960000	0.327982000
H	2.365779000	-2.015929000	-2.331103000
C	-4.146117000	1.116743000	0.060967000
C	-5.000068000	0.142675000	-0.456515000
C	-4.534244000	1.958462000	1.103336000
C	-6.272952000	0.039085000	0.092775000
C	-5.816808000	1.814505000	1.618051000
C	-6.700561000	0.861662000	1.127124000
H	-6.949572000	-0.711823000	-0.304031000
H	-6.129715000	2.463325000	2.430608000
C	-3.594381000	2.977121000	1.673057000
H	-2.640019000	2.520628000	1.946461000
H	-3.372524000	3.774066000	0.958056000
H	-4.023331000	3.437048000	2.563615000
C	-4.565161000	-0.785880000	-1.546779000
H	-4.031516000	-0.258996000	-2.340745000
H	-3.889272000	-1.548986000	-1.148599000
H	-5.428003000	-1.287479000	-1.986603000
C	1.202557000	2.293579000	0.642212000
H	0.912096000	3.161106000	0.043470000
H	0.366996000	2.075385000	1.311799000

H	2.063533000	2.577789000	1.247600000
C	-0.245313000	-1.387991000	-2.490195000
H	-0.862036000	-1.982401000	-1.808953000
H	-0.909322000	-0.695809000	-3.012164000
H	0.197780000	-2.060374000	-3.225814000
C	4.553515000	-1.026969000	-1.064741000
H	4.988030000	-1.080826000	-0.063842000
H	4.600765000	-2.021937000	-1.509307000
H	5.191754000	-0.366368000	-1.659286000
C	-8.068343000	0.702146000	1.719229000
H	-8.070220000	-0.075639000	2.489161000
H	-8.410959000	1.626847000	2.186693000
H	-8.798422000	0.410604000	0.961713000
H	-1.927678000	-1.344659000	0.290457000
H	-0.520386000	2.638215000	-2.307447000
O	-2.052005000	-2.324504000	0.378351000
C	-1.880480000	-2.677034000	1.723326000
H	-2.749027000	-3.238978000	2.087169000
H	-0.992597000	-3.308772000	1.857239000
H	-1.760633000	-1.794886000	2.364188000

IMes-TS1-A ν_{198} cm⁻¹ Etot = -1382.160342678691 a.u.

H	-1.133283000	4.105039000	0.521818000
C	-2.035729000	2.195176000	1.176918000
C	-1.207888000	3.030687000	0.518599000
N	-1.684356000	0.916042000	0.787231000
C	-0.666327000	0.927595000	-0.099961000
N	-0.379505000	2.236553000	-0.252078000
H	-2.832443000	2.387973000	1.875336000
H	2.120333000	-0.506783000	1.428574000
O	2.207038000	-0.564833000	2.409366000
C	0.669639000	-0.734008000	-0.534358000
O	1.807629000	-0.356121000	-0.223873000
C	0.613782000	2.770334000	-1.135199000
C	1.861790000	3.120188000	-0.621570000
C	0.281735000	2.958805000	-2.475066000
C	2.788824000	3.667130000	-1.499947000
C	1.244890000	3.508720000	-3.312054000
C	2.503971000	3.863652000	-2.845506000
H	3.766815000	3.942228000	-1.117080000
H	1.000030000	3.664935000	-4.358359000
C	-2.352540000	-0.265680000	1.238879000
C	-3.320167000	-0.839604000	0.412886000
C	-2.041258000	-0.790333000	2.494063000
C	-3.965942000	-1.983951000	0.863760000

C	-2.722373000	-1.933811000	2.899358000
C	-3.676991000	-2.549266000	2.100393000
H	-4.723687000	-2.438998000	0.233055000
H	-2.493560000	-2.353997000	3.873931000
C	3.540075000	4.420718000	-3.774219000
H	4.201782000	3.627567000	-4.135872000
H	3.082772000	4.890418000	-4.646758000
H	4.166057000	5.162464000	-3.274365000
C	2.206442000	2.901418000	0.817732000
H	1.485343000	3.376810000	1.487486000
H	2.216638000	1.835570000	1.057185000
H	3.192707000	3.309330000	1.039856000
C	-1.002367000	-0.173004000	3.377596000
H	0.011186000	-0.355351000	3.003287000
H	-1.123811000	0.909304000	3.457134000
H	-1.064055000	-0.594337000	4.381629000
C	-3.662889000	-0.241384000	-0.917081000
H	-3.929390000	0.814666000	-0.824541000
H	-2.816938000	-0.298342000	-1.607052000
H	-4.506052000	-0.766534000	-1.366600000
C	-4.365056000	-3.801762000	2.552113000
H	-3.802818000	-4.687272000	2.239778000
H	-4.451917000	-3.838293000	3.639399000
H	-5.366145000	-3.883267000	2.124945000
C	-1.065114000	2.576716000	-3.007577000
H	-1.200013000	1.491910000	-2.993786000
H	-1.873892000	3.008594000	-2.412560000
H	-1.180649000	2.918075000	-4.036622000
H	0.057219000	-1.334193000	0.158660000
C	0.309500000	-1.001606000	-1.938070000
C	-0.587634000	-1.867771000	-2.484066000
O	1.000197000	-0.377108000	-2.916415000
C	-0.441433000	-1.758203000	-3.895837000
H	-1.258179000	-2.512972000	-1.938003000
C	0.535002000	-0.838693000	-4.093627000
H	-0.978885000	-2.297256000	-4.659667000
H	0.995540000	-0.429292000	-4.977624000
C	3.308246000	-1.372032000	2.721114000
H	4.250554000	-0.960816000	2.334447000
H	3.391041000	-1.432334000	3.809228000
H	3.202981000	-2.394926000	2.334093000

IMes-II-A

Etot = -1382.186706583253 a.u.

C	-0.527010000	-0.450921000	-0.138198000
C	-1.221480000	-2.294697000	-1.176261000

H	-1.933254000	-2.956746000	-1.637631000
C	0.103516000	-2.417050000	-0.959703000
H	0.793273000	-3.208592000	-1.195630000
N	-1.595653000	-1.068292000	-0.668500000
N	0.521982000	-1.269282000	-0.321890000
C	1.888734000	-1.037670000	0.056298000
C	2.739299000	-0.467380000	-0.896607000
C	2.330990000	-1.441606000	1.311455000
C	4.062946000	-0.269899000	-0.543066000
C	3.672527000	-1.212839000	1.613968000
C	4.545627000	-0.624865000	0.714584000
H	4.736038000	0.179107000	-1.266873000
H	4.033340000	-1.503898000	2.595460000
C	-2.941549000	-0.572577000	-0.683062000
C	-3.777490000	-0.882683000	0.389428000
C	-3.367191000	0.172734000	-1.781061000
C	-5.087396000	-0.422536000	0.327771000
C	-4.686609000	0.606632000	-1.790971000
C	-5.559342000	0.320905000	-0.747375000
H	-5.755637000	-0.649817000	1.152396000
H	-5.038726000	1.188369000	-2.637125000
C	-2.431642000	0.524966000	-2.896564000
H	-1.641717000	1.196891000	-2.547342000
H	-1.942183000	-0.358238000	-3.314724000
H	-2.968219000	1.027259000	-3.701386000
C	-3.274062000	-1.650622000	1.570473000
H	-2.927803000	-2.647604000	1.281352000
H	-2.426679000	-1.123784000	2.028191000
H	-4.063978000	-1.771492000	2.311724000
C	2.245936000	-0.084858000	-2.258633000
H	1.857560000	-0.949163000	-2.805399000
H	1.442369000	0.652310000	-2.199854000
H	3.055571000	0.346185000	-2.847399000
C	1.454142000	-2.099233000	2.329597000
H	1.369771000	-1.458224000	3.211017000
H	0.443976000	-2.273476000	1.966439000
H	1.892214000	-3.052851000	2.637779000
C	5.972872000	-0.357877000	1.084276000
H	6.118899000	0.701038000	1.317695000
H	6.271372000	-0.933317000	1.961436000
H	6.650168000	-0.605446000	0.263786000
C	-6.968019000	0.831398000	-0.765666000
H	-7.027161000	1.816978000	-0.293741000
H	-7.341859000	0.934518000	-1.785774000
H	-7.639378000	0.167391000	-0.218698000
C	-0.630980000	0.781228000	0.752121000

O	-0.664592000	0.300835000	2.001300000
H	0.315883000	0.592403000	3.236509000
C	0.432450000	1.804368000	0.457096000
C	1.425886000	2.341403000	1.203246000
O	0.373190000	2.420946000	-0.758783000
C	2.029966000	3.350819000	0.393131000
H	1.680636000	2.043257000	2.209440000
C	1.356149000	3.354831000	-0.778957000
H	2.854748000	3.994343000	0.656097000
H	1.441533000	3.935085000	-1.683006000
O	0.919966000	0.716141000	4.023304000
C	0.210237000	1.376964000	5.028830000
H	0.872308000	1.518280000	5.888348000
H	-0.143871000	2.368708000	4.711730000
H	-0.665234000	0.806027000	5.370271000
H	-1.583062000	1.260680000	0.422406000

IMes-TS2-A $\nu_{361} \text{ cm}^{-1}$ Etot = -1382.154530777847

C	-0.393455000000	-0.295381000000	0.082781000000
C	-1.203416000000	-2.269081000000	-0.561610000000
H	-1.970557000000	-2.988377000000	-0.788779000000
C	0.137855000000	-2.350658000000	-0.608408000000
H	0.793801000000	-3.153739000000	-0.895639000000
N	-1.526820000000	-0.993580000000	-0.137749000000
N	0.632425000000	-1.125772000000	-0.212322000000
C	2.021807000000	-0.776816000000	-0.283998000000
C	2.868242000000	-1.156386000000	0.757593000000
C	2.485872000000	-0.137573000000	-1.435541000000
C	4.212823000000	-0.828191000000	0.647875000000
C	3.841214000000	0.168092000000	-1.489393000000
C	4.714728000000	-0.154161000000	-0.459187000000
H	4.885187000000	-1.109392000000	1.452351000000
H	4.222714000000	0.668802000000	-2.373653000000
C	-2.902053000000	-0.582768000000	-0.028285000000
C	-3.556570000000	-0.746449000000	1.188661000000
C	-3.547904000000	-0.123077000000	-1.174342000000
C	-4.907291000000	-0.431029000000	1.243664000000
C	-4.900279000000	0.180231000000	-1.063034000000
C	-5.595516000000	0.036920000000	0.130704000000
H	-5.433060000000	-0.549297000000	2.186197000000
H	-5.422065000000	0.544256000000	-1.942665000000
C	-2.816558000000	0.088717000000	-2.462024000000
H	-2.118816000000	0.935315000000	-2.380687000000
H	-2.235362000000	-0.791156000000	-2.751575000000
H	-3.521559000000	0.303168000000	-3.265850000000

C	-2.824630000000	-1.192553000000	2.415272000000
H	-2.200606000000	-2.070457000000	2.230935000000
H	-2.170383000000	-0.392008000000	2.772971000000
H	-3.524603000000	-1.435399000000	3.214968000000
C	2.359389000000	-1.905072000000	1.949893000000
H	1.573576000000	-1.343021000000	2.458817000000
H	1.941211000000	-2.876236000000	1.670599000000
H	3.165548000000	-2.080232000000	2.662176000000
C	1.583489000000	0.189856000000	-2.583542000000
H	1.000604000000	-0.683707000000	-2.889853000000
H	0.864822000000	0.987186000000	-2.345692000000
H	2.173076000000	0.514358000000	-3.441295000000
C	6.161795000000	0.227199000000	-0.532220000000
H	6.792752000000	-0.497827000000	-0.014805000000
H	6.502193000000	0.303837000000	-1.566112000000
H	6.327977000000	1.200563000000	-0.060204000000
C	-7.044826000000	0.406680000000	0.224733000000
H	-7.157763000000	1.452267000000	0.527528000000
H	-7.549368000000	0.288816000000	-0.735756000000
H	-7.565892000000	-0.204985000000	0.963599000000
C	-0.272018000000	1.127648000000	0.416126000000
O	-1.527516000000	1.711209000000	0.663471000000
C	0.726932000000	1.446964000000	1.463960000000
H	-1.630317000000	2.252311000000	-0.158619000000
C	0.798742000000	1.187456000000	2.797419000000
O	1.751705000000	2.267960000000	1.113235000000
C	1.938399000000	1.881901000000	3.292155000000
H	0.100152000000	0.592749000000	3.365005000000
C	2.473836000000	2.515733000000	2.221082000000
H	2.305665000000	1.912543000000	4.305645000000
H	3.332032000000	3.154914000000	2.095262000000
H	-0.034581000000	1.691090000000	-0.633189000000
O	-0.670736000000	2.434046000000	-1.707815000000
C	-0.168260000000	3.682561000000	-2.010115000000
H	0.288410000000	4.191585000000	-1.140592000000
H	0.615281000000	3.649730000000	-2.791280000000
H	-0.950667000000	4.364054000000	-2.388075000000

IMes-III-A

Etot = -1382.178302038680 a.u.

C	-0.381303000	-0.295151000	-0.121930000
C	-1.148420000	-2.237324000	-0.995525000
H	-1.888505000	-2.958547000	-1.296099000
C	0.182396000	-2.244451000	-1.123072000
H	0.847748000	-2.993256000	-1.515764000
N	-1.516056000	-1.047437000	-0.378251000

N	0.677164000	-1.059338000	-0.583861000
C	2.054025000	-0.919784000	-0.245008000
C	2.969455000	-0.644997000	-1.262528000
C	2.465840000	-1.135657000	1.071582000
C	4.315722000	-0.568222000	-0.932335000
C	3.823495000	-1.031858000	1.353911000
C	4.762169000	-0.744641000	0.372022000
H	5.035125000	-0.353820000	-1.717195000
H	4.155246000	-1.198637000	2.374415000
C	-2.865340000	-0.589935000	-0.357012000
C	-3.728141000	-1.061463000	0.632716000
C	-3.304640000	0.275269000	-1.361059000
C	-5.050406000	-0.633240000	0.603675000
C	-4.632294000	0.685780000	-1.339157000
C	-5.519947000	0.245808000	-0.364297000
H	-5.730946000	-0.994554000	1.368781000
H	-4.984541000	1.356480000	-2.117499000
C	-2.377420000	0.739730000	-2.442379000
H	-1.567804000	1.355290000	-2.039757000
H	-1.905164000	-0.106109000	-2.949596000
H	-2.917047000	1.325751000	-3.186846000
C	-3.245626000	-1.976232000	1.715230000
H	-2.717697000	-2.843769000	1.312995000
H	-2.553020000	-1.460425000	2.386346000
H	-4.083796000	-2.335490000	2.313117000
C	2.513646000	-0.416205000	-2.670309000
H	2.073512000	-1.314761000	-3.111639000
H	1.751122000	0.364946000	-2.704885000
H	3.350859000	-0.112308000	-3.299635000
C	1.493252000	-1.496497000	2.150002000
H	0.870248000	-0.645695000	2.436823000
H	0.812466000	-2.287286000	1.824708000
H	2.020265000	-1.845109000	3.038617000
C	6.215481000	-0.610135000	0.713002000
H	6.458787000	0.424693000	0.973631000
H	6.483000000	-1.232671000	1.568784000
H	6.850873000	-0.893234000	-0.128274000
C	-6.941411000	0.721681000	-0.348204000
H	-7.034092000	1.654404000	0.217002000
H	-7.308382000	0.915517000	-1.357927000
H	-7.600990000	-0.010320000	0.120976000
C	-0.356822000	0.932910000	0.494667000
O	-1.470909000	1.253725000	1.274934000
H	-1.470691000	0.675085000	3.031811000
C	0.673654000	1.921878000	0.502338000
C	0.879428000	2.990048000	1.339221000

O	1.574272000	1.970922000	-0.515541000
C	1.978972000	3.717079000	0.801155000
H	0.325610000	3.206409000	2.237934000
C	2.368919000	3.054808000	-0.310447000
H	2.428543000	4.612910000	1.199717000
H	3.160016000	3.201320000	-1.026035000
O	-1.426548000	0.224824000	3.889716000
C	-0.784834000	1.066080000	4.811964000
H	-0.734300000	0.537791000	5.765901000
H	0.240438000	1.316662000	4.508626000
H	-1.333844000	2.003334000	4.975573000
H	-1.909323000	2.032268000	0.913994000

IMes-IV-A

Etot = -1725.290133585273 a.u.

C	0.582086000	-1.575875000	-0.379342000
C	-0.486386000	0.379897000	-0.313373000
C	0.792539000	0.602292000	0.038469000
H	1.309169000	1.500594000	0.328259000
N	-0.614278000	-0.967993000	-0.564832000
N	1.440969000	-0.608229000	0.001332000
C	2.812311000	-0.684775000	0.455362000
C	3.844642000	-0.437248000	-0.440280000
C	3.027318000	-0.870722000	1.822110000
C	5.141366000	-0.423772000	0.065854000
C	4.338765000	-0.848306000	2.270358000
C	5.410903000	-0.637523000	1.408816000
H	5.962255000	-0.238898000	-0.619875000
H	4.527328000	-1.004851000	3.327870000
C	-1.946344000	-1.502686000	-0.760417000
C	-2.522344000	-1.515706000	-2.026410000
C	-2.668293000	-1.846212000	0.392654000
C	-3.832830000	-1.977783000	-2.132483000
C	-3.969254000	-2.292665000	0.224466000
C	-4.563969000	-2.387366000	-1.030248000
H	-4.291231000	-2.004130000	-3.116029000
H	-4.534087000	-2.578417000	1.105908000
C	-2.065684000	-1.763837000	1.759139000
H	-1.265573000	-2.507494000	1.886317000
H	-1.635353000	-0.776530000	1.951196000
H	-2.827516000	-1.949510000	2.515971000
C	-1.820657000	-1.053244000	-3.265159000
H	-1.066406000	-0.292821000	-3.058914000
H	-1.323653000	-1.888170000	-3.764064000
H	-2.542350000	-0.628842000	-3.964554000
C	3.607024000	-0.211856000	-1.900536000

H	3.351624000	-1.148162000	-2.403141000
H	2.786509000	0.486848000	-2.083051000
H	4.502682000	0.192738000	-2.372310000
C	1.894658000	-1.107195000	2.770972000
H	1.201656000	-0.260112000	2.789664000
H	1.316404000	-1.994553000	2.493830000
H	2.271166000	-1.248212000	3.783897000
C	6.818382000	-0.658078000	1.921609000
H	6.898412000	-0.153237000	2.886619000
H	7.161471000	-1.687165000	2.064440000
H	7.504383000	-0.175293000	1.224136000
C	-5.956170000	-2.918598000	-1.176018000
H	-5.961145000	-4.008535000	-1.082422000
H	-6.615408000	-2.524597000	-0.399722000
H	-6.380577000	-2.667122000	-2.148831000
H	-1.332904000	1.039819000	-0.388955000
C	0.998940000	-3.043133000	-0.563617000
O	2.137768000	-3.264187000	0.186041000
C	1.297782000	-3.285924000	-2.007464000
C	-0.107386000	-4.001902000	0.143886000
H	1.677686000	-3.644984000	1.020979000
C	1.220267000	-2.533523000	-3.137922000
O	1.837884000	-4.486271000	-2.302706000
O	0.226441000	-3.962202000	1.453693000
H	-1.091713000	-3.574617000	-0.090701000
C	-0.121667000	-5.383072000	-0.427271000
C	1.728933000	-3.339322000	-4.199048000
H	0.871711000	-1.517964000	-3.210117000
C	2.086856000	-4.511364000	-3.625394000
C	0.335605000	-6.572350000	0.033020000
O	-0.756684000	-5.555933000	-1.617341000
H	1.821231000	-3.076757000	-5.240719000
H	2.516311000	-5.423046000	-4.005874000
C	-0.025510000	-7.543611000	-0.947505000
H	0.836384000	-6.730727000	0.974555000
C	-0.679560000	-6.871549000	-1.923116000
H	0.167667000	-8.604547000	-0.921708000
H	-1.143150000	-7.171762000	-2.848452000
H	0.123062000	-5.189571000	2.628466000
O	0.199704000	-5.836154000	3.369343000
C	1.030886000	-5.278650000	4.340925000
H	2.037446000	-5.047753000	3.959764000
H	0.618693000	-4.353389000	4.772982000
H	1.143773000	-6.000262000	5.155203000

IMes-V-A

Etot = -1725.295087097841 a.u.

C	0.338952000	-1.457487000	-0.138568000
C	-0.691190000	0.524824000	-0.055358000
C	0.621558000	0.741481000	0.136600000
H	1.178443000	1.645663000	0.310246000
N	-0.856312000	-0.834097000	-0.228835000
N	1.246494000	-0.479570000	0.079779000
C	2.673460000	-0.582935000	0.247860000
C	3.484171000	-0.375700000	-0.868085000
C	3.191604000	-0.747255000	1.533007000
C	4.859548000	-0.440634000	-0.683168000
C	4.573208000	-0.809331000	1.656692000
C	5.421118000	-0.678067000	0.564673000
H	5.506750000	-0.300174000	-1.543187000
H	4.992681000	-0.975544000	2.643205000
C	-2.179702000	-1.344617000	-0.473309000
C	-2.616667000	-1.465854000	-1.792638000
C	-3.015287000	-1.572983000	0.616626000
C	-3.925427000	-1.877090000	-2.002507000
C	-4.316236000	-1.982308000	0.349606000
C	-4.786471000	-2.150847000	-0.945280000
H	-4.280591000	-1.985652000	-3.022501000
H	-4.977941000	-2.182271000	1.186203000
C	-2.557516000	-1.355812000	2.024365000
H	-1.546374000	-1.730515000	2.181651000
H	-2.565848000	-0.291122000	2.280327000
H	-3.220487000	-1.868801000	2.720607000
C	-1.712312000	-1.182187000	-2.952440000
H	-1.193173000	-0.226794000	-2.844471000
H	-0.946384000	-1.956013000	-3.056451000
H	-2.281181000	-1.156558000	-3.881661000
C	2.916130000	-0.039721000	-2.212544000
H	3.700965000	-0.049364000	-2.968751000
H	2.149638000	-0.753402000	-2.516675000
H	2.465039000	0.957832000	-2.213977000
C	2.315028000	-0.804004000	2.742793000
H	1.891771000	0.183299000	2.959012000
H	1.499704000	-1.512811000	2.591077000
H	2.888934000	-1.127331000	3.609904000
C	6.904970000	-0.799234000	0.732285000
H	7.247261000	-0.284177000	1.632306000
H	7.195905000	-1.849345000	0.831654000
H	7.439576000	-0.385806000	-0.124357000
C	-6.180013000	-2.637032000	-1.201199000
H	-6.186206000	-3.720599000	-1.353240000
H	-6.838808000	-2.420307000	-0.359066000

H	-6.604224000	-2.179634000	-2.097108000
H	-1.531772000	1.195410000	-0.089198000
C	0.694061000	-2.971989000	-0.026190000
O	1.005188000	-3.159142000	1.262312000
C	1.808054000	-3.282132000	-1.007071000
C	-0.563431000	-3.906532000	-0.358103000
H	-0.542772000	-3.801465000	1.483736000
C	1.880448000	-3.320620000	-2.365687000
O	2.979440000	-3.691327000	-0.480435000
O	-1.275100000	-3.989011000	0.835484000
H	-1.188555000	-3.468883000	-1.141583000
C	-0.151549000	-5.255852000	-0.844242000
C	3.190282000	-3.777322000	-2.688482000
H	1.086730000	-3.092577000	-3.059218000
C	3.807228000	-3.985974000	-1.501395000
C	0.440731000	-6.322186000	-0.252135000
O	-0.424873000	-5.543791000	-2.143410000
H	3.608388000	-3.941167000	-3.668984000
H	4.790259000	-4.330410000	-1.227112000
C	0.548645000	-7.330542000	-1.254090000
H	0.760539000	-6.373881000	0.775782000
C	0.010206000	-6.802650000	-2.377520000
H	0.968075000	-8.318643000	-1.149429000
H	-0.140120000	-7.179498000	-3.375478000
H	2.410484000	-3.706082000	2.152360000
O	3.110302000	-3.963548000	2.790076000
C	3.290872000	-5.346038000	2.713029000
H	2.394515000	-5.907373000	3.017336000
H	3.569209000	-5.680293000	1.703315000
H	4.100173000	-5.625073000	3.393649000

VI...IMes-I(H)-A

Etot = -1725.297972868944a.u.

C	-1.852282000	0.626239000	-0.170397000
C	-2.603389000	2.195411000	-1.629824000
H	-3.331070000	2.837764000	-2.096109000
C	-1.293137000	2.008854000	-1.885726000
N	-2.918861000	1.349916000	-0.582926000
N	-0.858693000	1.054253000	-0.985178000
C	0.481710000	0.567323000	-0.916893000
C	1.462438000	1.361278000	-0.319847000
C	0.770233000	-0.693556000	-1.440762000
C	2.758350000	0.860048000	-0.265977000
C	2.080801000	-1.149976000	-1.357026000
C	3.088512000	-0.388053000	-0.778433000
H	3.529524000	1.463935000	0.202580000

H	2.317797000	-2.130114000	-1.760194000
C	-4.224956000	1.249848000	-0.010754000
C	-5.008556000	0.134847000	-0.301353000
C	-4.680378000	2.278634000	0.817040000
C	-6.282095000	0.071377000	0.254556000
C	-5.960682000	2.167783000	1.343492000
C	-6.775746000	1.073494000	1.077390000
H	-6.903944000	-0.790741000	0.033200000
H	-6.326734000	2.960117000	1.989664000
C	-3.815902000	3.452493000	1.161258000
H	-2.904401000	3.141818000	1.680853000
H	-3.505018000	4.007388000	0.272459000
H	-4.356468000	4.140866000	1.811837000
C	-4.505031000	-0.979200000	-1.166270000
H	-4.001805000	-0.603879000	-2.060021000
H	-3.783609000	-1.595028000	-0.622053000
H	-5.329826000	-1.620327000	-1.479688000
C	1.137801000	2.697779000	0.273405000
H	0.711294000	3.378120000	-0.467904000
H	0.410179000	2.617617000	1.086473000
H	2.039358000	3.162222000	0.674302000
C	-0.295134000	-1.544998000	-2.060374000
H	-0.996205000	-1.907659000	-1.303578000
H	-0.879919000	-0.985238000	-2.794122000
H	0.147363000	-2.407409000	-2.559889000
C	4.500796000	-0.888940000	-0.732776000
H	5.048190000	-0.458074000	0.107534000
H	4.536051000	-1.976493000	-0.644146000
H	5.039880000	-0.619817000	-1.646539000
C	-8.141868000	0.971621000	1.686025000
H	-8.077789000	0.693019000	2.742256000
H	-8.672969000	1.924773000	1.634589000
H	-8.746771000	0.216608000	1.181603000
H	-0.643798000	2.455918000	-2.619298000
H	-1.873132000	-0.823189000	0.929443000
O	-1.901761000	-1.723040000	1.384692000
C	-0.720894000	-1.932132000	2.066817000
C	-0.389420000	-0.752541000	3.003787000
H	0.144180000	-2.058642000	1.393957000
C	-0.842313000	-3.178646000	2.881994000
O	-1.239260000	0.051797000	3.320780000
C	0.984951000	-0.643125000	3.479736000
C	-1.874697000	-3.708455000	3.581930000
O	0.250493000	-3.974114000	2.986714000
C	2.130623000	-1.339618000	3.215325000
O	1.256369000	0.358561000	4.357776000

C	-1.385274000	-4.917796000	4.157567000
H	-2.862154000	-3.283792000	3.656234000
C	-0.094408000	-5.025234000	3.767496000
C	3.157370000	-0.730648000	3.975848000
H	2.220181000	-2.189851000	2.559714000
C	2.561055000	0.291496000	4.644703000
H	-1.925417000	-5.615616000	4.777416000
H	0.676317000	-5.756672000	3.944043000
H	4.197351000	-1.010266000	4.023890000
H	2.932623000	1.028817000	5.338037000
O	-0.944808000	2.834988000	3.162637000
C	-0.809267000	3.474532000	4.404619000
H	-1.060190000	1.883151000	3.317451000
H	-1.702531000	3.359112000	5.032010000
H	0.055382000	3.104070000	4.970321000
H	-0.662188000	4.540327000	4.217971000

VI Etot = -686.227229359367 a.u.

C	-0.322889000	0.283390000	0.276329000
C	0.367040000	-0.981073000	0.021926000
C	-0.050287000	-2.211208000	-0.404561000
O	1.705419000	-1.005581000	0.236292000
C	1.102237000	-3.032929000	-0.451376000
H	-1.061286000	-2.497257000	-0.646053000
C	2.131839000	-2.240870000	-0.052443000
H	1.162284000	-4.068981000	-0.742769000
H	3.188470000	-2.417551000	0.067775000
O	0.256387000	1.280651000	0.620664000
C	-1.852216000	0.247850000	0.110150000
H	-2.093916000	-0.414134000	-0.732379000
O	-2.284554000	1.558570000	-0.136507000
H	-3.199096000	1.626666000	0.149061000
C	-2.460203000	-0.346685000	1.335234000
C	-2.511574000	0.061000000	2.629470000
O	-3.114721000	-1.527655000	1.194684000
C	-3.250176000	-0.933638000	3.332294000
H	-2.066265000	0.960300000	3.024575000
C	-3.583439000	-1.871369000	2.414904000
H	-3.495312000	-0.949138000	4.382107000
H	-4.131805000	-2.797087000	2.467775000

IMes-I(H2)-B Etot = -1154.185637114467

C	-0.276715000000	-0.567668000000	0.295649000000
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C	-0.711310000000	1.493048000000	-0.558582000000
H	-1.368378000000	2.281508000000	-0.894392000000
C	0.648104000000	1.418919000000	-0.564338000000
H	1.857265000000	2.622444000000	-0.890020000000
N	-1.249959000000	0.304736000000	-0.038058000000
N	0.847342000000	0.129406000000	-0.023460000000
C	2.141488000000	-0.423184000000	0.170547000000
C	2.990089000000	0.133272000000	1.132013000000
C	2.560004000000	-1.502438000000	-0.611925000000
C	4.251088000000	-0.424773000000	1.309320000000
C	3.831128000000	-2.026762000000	-0.398770000000
C	4.689807000000	-1.508091000000	0.560005000000
H	4.910047000000	0.007966000000	2.057799000000
H	4.159228000000	-2.861594000000	-1.012993000000
C	-2.633680000000	0.058312000000	0.133407000000
C	-3.294886000000	-0.833972000000	-0.713869000000
C	-3.327502000000	0.740663000000	1.137747000000
C	-4.663252000000	-1.018990000000	-0.543051000000
C	-4.694179000000	0.525765000000	1.269264000000
C	-5.381563000000	-0.350379000000	0.438516000000
H	-5.181042000000	-1.708783000000	-1.204398000000
H	-5.233288000000	1.054154000000	2.051435000000
C	-2.606181000000	1.657562000000	2.077122000000
H	-1.752341000000	1.147481000000	2.530089000000
H	-2.200712000000	2.531100000000	1.561563000000
H	-3.274044000000	1.999147000000	2.870203000000
C	-2.553196000000	-1.589161000000	-1.771736000000
H	-1.832550000000	-0.948523000000	-2.283656000000
H	-1.988700000000	-2.413690000000	-1.327397000000
H	-3.248369000000	-2.001062000000	-2.506573000000
C	2.566475000000	1.313038000000	1.948857000000
H	2.565391000000	2.218131000000	1.334577000000
H	1.550096000000	1.184958000000	2.327666000000
H	3.244817000000	1.456330000000	2.793207000000
C	1.676962000000	-2.083890000000	-1.672713000000
H	0.893053000000	-2.706237000000	-1.232060000000
H	1.180853000000	-1.294068000000	-2.240819000000
H	2.263711000000	-2.697564000000	-2.360253000000
C	6.043181000000	-2.112711000000	0.794988000000
H	6.004916000000	-2.886692000000	1.569497000000
H	6.432007000000	-2.580581000000	-0.112643000000
H	6.763788000000	-1.359746000000	1.123186000000
C	-6.850991000000	-0.593268000000	0.621227000000
H	-7.033193000000	-1.377337000000	1.363985000000
H	-7.364543000000	0.307125000000	0.966889000000
H	-7.319429000000	-0.914069000000	-0.311910000000

O	2.509751000000	3.419797000000	-0.968381000000
C	1.740421000000	4.569787000000	-1.048786000000
H	2.311166000000	5.431676000000	-0.675769000000
H	1.430155000000	4.811921000000	-2.081850000000
H	0.819579000000	4.500745000000	-0.446759000000
H	-0.530044000000	-2.316246000000	0.651941000000
O	-0.661719000000	-3.318062000000	0.737503000000
C	0.109574000000	-3.762601000000	1.808149000000
H	-0.227150000000	-3.352609000000	2.774159000000
H	0.033664000000	-4.854243000000	1.871160000000
H	1.175247000000	-3.508813000000	1.699677000000

IMes-I-B

Etot = --922.867346068235a.u.

C	-0.014727000	-0.000178000	-0.278469000
C	0.649041000	0.000884000	1.898187000
H	1.397530000	0.001190000	2.678780000
C	-0.715533000	0.001071000	1.979988000
N	1.049461000	0.000134000	0.553717000
N	-1.052078000	0.000392000	0.605085000
C	-2.403365000	0.000108000	0.159092000
C	-3.063613000	1.214319000	-0.045133000
C	-3.062718000	-1.214560000	-0.046187000
C	-4.392158000	1.191760000	-0.460604000
C	-4.391151000	-1.192751000	-0.461632000
C	-5.074068000	-0.000621000	-0.677995000
H	-4.908133000	2.135624000	-0.614609000
H	-4.906329000	-2.136936000	-0.616411000
C	2.403261000	-0.000080000	0.121264000
C	3.064824000	-1.216365000	-0.068345000
C	3.063900000	1.216257000	-0.072310000
C	4.399217000	-1.193053000	-0.462975000
C	4.398157000	1.192835000	-0.466853000
C	5.083521000	-0.000224000	-0.670711000
H	4.917777000	-2.136574000	-0.608629000
H	4.915877000	2.136355000	-0.615556000
C	2.354592000	2.519524000	0.135473000
H	1.510696000	2.620769000	-0.552343000
H	1.945493000	2.592689000	1.146461000
H	3.033853000	3.357537000	-0.024831000
C	2.356759000	-2.519651000	0.143555000
H	1.947805000	-2.590097000	1.154788000
H	1.512932000	-2.623909000	-0.543896000
H	3.036813000	-3.357505000	-0.014190000
C	-2.361288000	2.517288000	0.184517000
H	-1.972949000	2.577384000	1.204678000

H	-1.502314000	2.624900000	-0.483591000
H	-3.037659000	3.356449000	0.016734000
C	-2.359244000	-2.517092000	0.182430000
H	-1.500970000	-2.623966000	-0.486699000
H	-1.969682000	-2.577089000	1.202129000
H	-3.035233000	-3.356684000	0.015265000
C	-6.496347000	-0.001193000	-1.155196000
H	-6.541915000	-0.014672000	-2.249123000
H	-7.034854000	-0.881035000	-0.797313000
H	-7.028142000	0.891083000	-0.818928000
C	6.512762000	-0.000099000	-1.125293000
H	6.573841000	0.014435000	-2.218385000
H	7.045818000	0.879322000	-0.758649000
H	7.038396000	-0.893208000	-0.782017000

IMes-I(H)-B

Etot = -1038.534015965433 a.u.

C	-0.219624000	-0.645732000	0.232366000
C	-0.679649000	1.404847000	-0.674811000
H	-1.346713000	2.189943000	-1.000223000
C	0.679596000	1.346637000	-0.679340000
H	1.851760000	2.538936000	-1.051642000
N	-1.197922000	0.215617000	-0.126342000
N	0.893478000	0.065673000	-0.118714000
C	2.190570000	-0.474384000	0.074346000
C	3.062516000	0.118515000	0.991425000
C	2.593299000	-1.589143000	-0.667527000
C	4.328240000	-0.433870000	1.162165000
C	3.866399000	-2.108581000	-0.462315000
C	4.749322000	-1.549024000	0.451973000
H	5.004146000	0.029092000	1.876957000
H	4.178271000	-2.971581000	-1.045864000
C	-2.574901000	-0.053165000	0.044522000
C	-3.345422000	-0.436662000	-1.055070000
C	-3.157310000	0.098499000	1.305905000
C	-4.707110000	-0.657195000	-0.873492000
C	-4.520151000	-0.136700000	1.444601000
C	-5.313503000	-0.514272000	0.367553000
H	-5.307814000	-0.955874000	-1.728983000
H	-4.974736000	-0.016088000	2.424843000
C	-2.317240000	0.499993000	2.477102000
H	-1.554293000	-0.257783000	2.672166000
H	-1.779510000	1.429360000	2.271771000
H	-2.931463000	0.634945000	3.369790000
C	-2.703680000	-0.635974000	-2.392941000
H	-2.227339000	0.280085000	-2.749944000

H	-1.909521000	-1.384301000	-2.324491000
H	-3.437574000	-0.964537000	-3.131507000
C	2.657469000	1.327748000	1.773692000
H	2.643629000	2.210623000	1.128075000
H	1.648197000	1.213844000	2.175406000
H	3.353135000	1.499304000	2.598907000
C	1.682228000	-2.203525000	-1.684587000
H	0.801902000	-2.634303000	-1.202035000
H	1.314849000	-1.443956000	-2.380027000
H	2.204472000	-2.978333000	-2.250894000
C	6.106849000	-2.146928000	0.681373000
H	6.072952000	-2.938057000	1.438895000
H	6.505387000	-2.592203000	-0.233842000
H	6.818720000	-1.394270000	1.028513000
C	-6.777537000	-0.790299000	0.549537000
H	-6.948349000	-1.811906000	0.906026000
H	-7.222826000	-0.113536000	1.283104000
H	-7.322962000	-0.677249000	-0.390061000
O	2.511219000	3.336644000	-1.164127000
C	1.745026000	4.484033000	-1.282707000
H	2.313948000	5.358431000	-0.934911000
H	1.437589000	4.696008000	-2.323946000
H	0.821661000	4.434761000	-0.682015000

IMes-TS1-B $i65\text{ cm}^{-1}$ Etot = -1381.619043481830 a.u.

C	-1.748522000	-1.922574000	-0.166544000
C	-2.256709000	-0.083912000	-1.433986000
H	-2.939694000	0.639309000	-1.856933000
C	-0.899663000	-0.167467000	-1.516519000
H	2.531613000	3.090452000	-0.746615000
N	-2.745046000	-1.130673000	-0.626508000
N	-0.659700000	-1.313147000	-0.721985000
C	0.650340000	-1.819927000	-0.526551000
C	1.555896000	-1.105988000	0.263340000
C	1.030517000	-3.016762000	-1.136233000
C	2.844153000	-1.604138000	0.420511000
C	2.326885000	-3.484816000	-0.944602000
C	3.251392000	-2.790997000	-0.175886000
H	3.548009000	-1.042826000	1.029565000
H	2.621480000	-4.417550000	-1.419723000
C	-4.108296000	-1.335615000	-0.314637000
C	-4.955207000	-1.914056000	-1.262307000
C	-4.601876000	-0.928495000	0.928231000
C	-6.301583000	-2.072470000	-0.949487000
C	-5.952497000	-1.108996000	1.201858000

C	-6.819941000	-1.678542000	0.276996000
H	-6.960851000	-2.524412000	-1.686413000
H	-6.337484000	-0.790303000	2.167378000
C	-3.681643000	-0.319572000	1.938579000
H	-2.916025000	-1.041047000	2.234766000
H	-3.148344000	0.536077000	1.516418000
H	-4.233638000	0.006614000	2.822398000
C	-4.409796000	-2.381849000	-2.575845000
H	-3.978021000	-1.556145000	-3.146440000
H	-3.599946000	-3.098856000	-2.416849000
H	-5.190357000	-2.855013000	-3.174960000
C	1.137907000	0.158653000	0.944185000
H	0.760235000	0.881537000	0.217743000
H	0.317837000	-0.037008000	1.641852000
H	1.973278000	0.599921000	1.490339000
C	0.063801000	-3.777923000	-1.988990000
H	-0.782614000	-4.126220000	-1.392124000
H	-0.351257000	-3.132962000	-2.768560000
H	0.553133000	-4.633274000	-2.460616000
C	4.658416000	-3.289377000	-0.018346000
H	5.040397000	-3.094634000	0.987103000
H	4.721691000	-4.364519000	-0.202220000
H	5.337107000	-2.795438000	-0.722214000
C	-8.268201000	-1.890354000	0.608962000
H	-8.413679000	-2.811218000	1.184044000
H	-8.664163000	-1.068172000	1.210358000
H	-8.875351000	-1.971084000	-0.295428000
O	3.260915000	3.272378000	-0.126082000
C	2.717609000	3.942167000	0.974966000
H	3.534296000	4.180373000	1.662815000
H	2.226194000	4.884605000	0.694036000
H	1.984510000	3.331825000	1.520714000
C	0.549788000	2.235015000	-2.536654000
H	0.915317000	1.205714000	-2.605467000
O	1.037943000	3.075337000	-1.797418000
C	-0.552413000	2.540145000	-3.438641000
C	-1.268290000	1.752703000	-4.291804000
O	-0.962615000	3.831825000	-3.551344000
C	-2.169731000	2.611848000	-4.968702000
H	-1.180933000	0.679591000	-4.348148000
C	-1.936003000	3.856521000	-4.473800000
H	-2.906487000	2.345491000	-5.710061000
H	-2.372365000	4.821374000	-4.676650000

IMes-II-B Etot = -1381.681853228635 a.u.

C	-0.632100000	-0.587232000	0.631198000
C	0.521722000	-1.011287000	0.076613000
N	-1.662782000	-1.093932000	-0.146790000
C	-1.221060000	-1.852687000	-1.183569000
N	0.129308000	-1.779656000	-1.020253000
H	-0.793241000	0.062726000	1.474520000
O	0.722834000	2.535490000	0.262873000
C	1.951834000	-0.595537000	0.379300000
O	2.261234000	0.581184000	-0.210632000
H	1.329963000	1.712418000	0.089278000
C	1.146796000	3.560944000	-0.568099000
H	2.187225000	3.870931000	-0.370979000
H	1.090740000	3.299018000	-1.638672000
H	0.510395000	4.443453000	-0.416547000
H	2.594173000	-1.435141000	0.024889000
C	2.138788000	-0.560565000	1.877249000
C	2.319877000	0.472462000	2.736689000
O	2.149500000	-1.736636000	2.564099000
C	2.442336000	-0.101649000	4.038904000
H	2.342018000	1.509893000	2.445579000
C	2.331997000	-1.440665000	3.872441000
H	2.595119000	0.413105000	4.975433000
H	2.368743000	-2.278546000	4.549807000
C	-3.028889000	-0.778861000	0.073930000
C	-3.483297000	0.505505000	-0.236993000
C	-3.881703000	-1.741829000	0.612626000
C	-4.817115000	0.807013000	0.018065000
C	-5.208563000	-1.395392000	0.843356000
C	-5.694407000	-0.126598000	0.555115000
H	-5.179060000	1.803814000	-0.219214000
H	-5.877389000	-2.139411000	1.267977000
C	1.026292000	-2.450242000	-1.900833000
C	1.604904000	-1.745705000	-2.958826000
C	1.301141000	-3.799460000	-1.687335000
C	2.466641000	-2.433507000	-3.805953000
C	2.168474000	-4.445983000	-2.561880000
C	2.758960000	-3.780093000	-3.627307000
H	2.926164000	-1.892403000	-4.628802000
H	2.390396000	-5.497290000	-2.398976000
C	1.316235000	-0.293062000	-3.154045000
H	0.240315000	-0.125570000	-3.255769000
H	1.657952000	0.273694000	-2.275169000
H	1.816804000	0.081803000	-4.048964000
C	0.680003000	-4.531499000	-0.538686000
H	0.937339000	-4.059609000	0.413626000

H	-0.410037000	-4.513881000	-0.616147000
H	1.017082000	-5.569409000	-0.513802000
C	3.674576000	-4.497774000	-4.575434000
H	4.030539000	-5.437524000	-4.147938000
H	3.165126000	-4.735102000	-5.515371000
H	4.546229000	-3.887664000	-4.825519000
C	-2.572022000	1.515838000	-0.862345000
H	-1.716352000	1.775946000	-0.231443000
H	-2.149064000	1.118969000	-1.789507000
H	-3.120248000	2.430384000	-1.095433000
C	-3.378661000	-3.114951000	0.932700000
H	-3.054342000	-3.624129000	0.022050000
H	-2.507759000	-3.072228000	1.591759000
H	-4.156041000	-3.708243000	1.417796000
C	-7.136636000	0.217267000	0.786812000
H	-7.734181000	0.044382000	-0.114642000
H	-7.567352000	-0.391521000	1.584922000
H	-7.256414000	1.268418000	1.058930000

IMes-TS2-B

*i*1088 cm⁻¹

Etot = -1381.643675343781 a.u.

C	-0.423755000	-0.811503000	0.530445000
C	0.728042000	-1.076344000	-0.139528000
N	-1.474396000	-1.125750000	-0.324857000
C	-1.055668000	-1.564206000	-1.534801000
N	0.300131000	-1.538887000	-1.393359000
H	-0.574121000	-0.439693000	1.527913000
O	3.486434000	-3.177624000	0.153150000
C	2.131176000	-1.016899000	0.306566000
O	3.004802000	-0.498624000	-0.692631000
H	3.611452000	-1.236790000	-0.855019000
C	4.218816000	-3.438962000	1.286652000
H	5.310993000	-3.343589000	1.124331000
H	3.977456000	-2.755361000	2.124476000
H	4.055309000	-4.464674000	1.673746000
H	2.667924000	-2.228040000	0.394241000
C	2.357994000	-0.293903000	1.560856000
C	3.294272000	0.637113000	1.910734000
O	1.611850000	-0.611189000	2.655556000
C	3.114255000	0.893401000	3.301954000
H	4.020608000	1.063601000	1.240236000
C	2.084615000	0.114373000	3.704008000
H	3.677924000	1.572509000	3.923904000
H	1.580128000	-0.029568000	4.644969000
C	-2.841042000	-1.019141000	0.036254000
C	-3.617869000	0.008222000	-0.503159000

C	-3.385278000	-1.937395000	0.936491000
C	-4.951016000	0.101300000	-0.120102000
C	-4.722206000	-1.801659000	1.295320000
C	-5.522262000	-0.791663000	0.777816000
H	-5.557926000	0.902324000	-0.533851000
H	-5.149889000	-2.515671000	1.994136000
C	1.124289000	-1.928355000	-2.494743000
C	1.492080000	-0.964715000	-3.435762000
C	1.483811000	-3.265336000	-2.648231000
C	2.242128000	-1.361665000	-4.533726000
C	2.237009000	-3.616846000	-3.766115000
C	2.629740000	-2.684905000	-4.713721000
H	2.530747000	-0.614365000	-5.268463000
H	2.523480000	-4.657536000	-3.890434000
C	1.098821000	0.465802000	-3.252116000
H	0.017776000	0.560182000	-3.121808000
H	1.577094000	0.868514000	-2.355352000
H	1.403586000	1.064691000	-4.112679000
C	1.104812000	-4.298612000	-1.637387000
H	1.774444000	-4.213260000	-0.771882000
H	0.074178000	-4.163203000	-1.303699000
H	1.209434000	-5.300621000	-2.059299000
C	3.472148000	-3.085387000	-5.889222000
H	3.195955000	-2.527208000	-6.787601000
H	4.533113000	-2.890968000	-5.699137000
H	3.369415000	-4.150961000	-6.105900000
C	-3.028464000	0.984134000	-1.472776000
H	-2.122746000	1.442739000	-1.067995000
H	-2.732852000	0.474618000	-2.392819000
H	-3.744947000	1.772427000	-1.711341000
C	-2.558758000	-3.062185000	1.478760000
H	-2.076395000	-3.611104000	0.666327000
H	-1.754449000	-2.702250000	2.124770000
H	-3.178639000	-3.753974000	2.051564000
C	-6.971778000	-0.687374000	1.151166000
H	-7.602588000	-1.236665000	0.444187000
H	-7.157791000	-1.102262000	2.144199000
H	-7.309820000	0.351450000	1.148214000

IMes-III-B

Etot = -1381.647909133304 a.u.

C	-0.535976000	-0.669463000	0.527620000
C	0.647304000	-0.918011000	-0.123954000
N	-1.564303000	-1.019714000	-0.350879000
C	-1.122277000	-1.461914000	-1.543557000
N	0.235600000	-1.400424000	-1.386339000

H	-0.715673000	-0.275921000	1.510196000
O	2.990395000	-3.431638000	0.856284000
C	2.002687000	-0.809900000	0.319456000
O	3.011791000	-0.727422000	-0.663116000
H	3.465706000	-1.576179000	-0.687044000
C	3.533300000	-3.587092000	2.139124000
H	4.200177000	-4.455031000	2.124026000
H	4.111087000	-2.709689000	2.454769000
H	2.760075000	-3.769850000	2.899228000
H	2.478133000	-2.577108000	0.838619000
C	2.369850000	-0.181355000	1.537080000
C	3.582637000	0.322570000	1.978613000
O	1.451656000	-0.058882000	2.543329000
C	3.376570000	0.752294000	3.317846000
H	4.485012000	0.375493000	1.393546000
C	2.082015000	0.503021000	3.623490000
H	4.104660000	1.200212000	3.978751000
H	1.470015000	0.668919000	4.493692000
C	-2.936487000	-0.944689000	-0.012066000
C	-3.736587000	0.042045000	-0.593186000
C	-3.467936000	-1.847598000	0.912088000
C	-5.077847000	0.106859000	-0.232587000
C	-4.813504000	-1.741027000	1.247281000
C	-5.636145000	-0.773348000	0.685656000
H	-5.701376000	0.877147000	-0.679118000
H	-5.229878000	-2.444931000	1.963258000
C	1.068201000	-1.797395000	-2.473141000
C	1.557964000	-0.829142000	-3.353093000
C	1.325188000	-3.150638000	-2.679258000
C	2.323233000	-1.238982000	-4.434953000
C	2.100582000	-3.517599000	-3.777641000
C	2.610686000	-2.580828000	-4.663077000
H	2.707337000	-0.486019000	-5.118711000
H	2.304681000	-4.572468000	-3.941058000
C	1.275278000	0.618765000	-3.114760000
H	0.205299000	0.788534000	-2.971767000
H	1.783633000	0.952880000	-2.206603000
H	1.621113000	1.225798000	-3.953868000
C	0.781333000	-4.190055000	-1.749726000
H	1.245043000	-4.115923000	-0.761793000
H	-0.296384000	-4.059813000	-1.624670000
H	0.975425000	-5.191059000	-2.140674000
C	3.447904000	-2.996138000	-5.837473000
H	3.014601000	-2.648148000	-6.780230000
H	4.457987000	-2.579443000	-5.774509000
H	3.538973000	-4.082832000	-5.892263000

C	-3.161068000	1.008791000	-1.580523000
H	-2.261644000	1.484754000	-1.181887000
H	-2.857434000	0.488695000	-2.491820000
H	-3.888651000	1.783399000	-1.831529000
C	-2.617577000	-2.928859000	1.502994000
H	-2.097584000	-3.480661000	0.715973000
H	-1.839985000	-2.521923000	2.153701000
H	-3.227305000	-3.626410000	2.080237000
C	-7.093536000	-0.700801000	1.035731000
H	-7.697728000	-1.298420000	0.344633000
H	-7.280306000	-1.080201000	2.042876000
H	-7.464110000	0.325775000	0.985850000

IMes-IV-B Etot = -1724.804512368608 a.u.

C	0.606255000	-1.506002000	-0.150116000
C	-0.537655000	0.493786000	-0.019970000
C	0.775988000	0.745691000	0.171984000
H	1.287498000	1.668519000	0.383404000
N	-0.606580000	-0.890848000	-0.217262000
N	1.440964000	-0.463991000	0.086183000
C	2.843714000	-0.601291000	0.275700000
C	3.676802000	-0.677695000	-0.839664000
C	3.354063000	-0.651818000	1.574678000
C	5.047764000	-0.787619000	-0.635223000
C	4.732695000	-0.758630000	1.728533000
C	5.594694000	-0.820135000	0.641027000
H	5.703156000	-0.851113000	-1.499641000
H	5.140192000	-0.803758000	2.734758000
C	-1.784848000	-1.685650000	-0.379031000
C	-2.226337000	-2.012276000	-1.656702000
C	-2.419030000	-2.182191000	0.760628000
C	-3.354431000	-2.819500000	-1.777601000
C	-3.539090000	-2.983493000	0.591978000
C	-4.030505000	-3.304104000	-0.668473000
H	-3.707637000	-3.075973000	-2.772810000
H	-4.043508000	-3.366708000	1.474981000
C	-1.891624000	-1.871403000	2.124382000
H	-0.886572000	-2.285463000	2.246845000
H	-1.812407000	-0.794050000	2.289423000
H	-2.538349000	-2.295027000	2.894517000
C	-1.500029000	-1.534046000	-2.874563000
H	-1.522823000	-0.443848000	-2.949974000
H	-0.449123000	-1.832984000	-2.836380000
H	-1.950165000	-1.950691000	-3.777523000
C	3.104813000	-0.659746000	-2.223212000

H	2.427048000	-1.504397000	-2.368689000
H	2.517836000	0.245621000	-2.399168000
H	3.898417000	-0.707626000	-2.970737000
C	2.445519000	-0.626353000	2.762750000
H	1.889992000	0.311759000	2.863038000
H	1.695229000	-1.417152000	2.682402000
H	3.014801000	-0.781010000	3.680925000
C	7.079577000	-0.898794000	0.841419000
H	7.515535000	0.099336000	0.955246000
H	7.330000000	-1.466071000	1.740704000
H	7.571416000	-1.375003000	-0.009537000
C	-5.269705000	-4.136233000	-0.820092000
H	-5.300804000	-4.944329000	-0.084740000
H	-6.170539000	-3.530835000	-0.674594000
H	-5.330288000	-4.580668000	-1.815926000
C	-1.705100000	1.460328000	-0.048454000
O	-2.878782000	0.856024000	0.389360000
H	-2.824271000	1.114905000	1.360873000
C	-1.872247000	1.997186000	-1.432713000
C	-1.009361000	2.161606000	-2.473260000
O	-3.079825000	2.508878000	-1.763054000
C	-1.737812000	2.824504000	-3.503511000
H	0.021192000	1.847338000	-2.490087000
C	-2.986288000	3.006982000	-3.012698000
H	-1.381693000	3.118056000	-4.478766000
H	-3.884442000	3.446904000	-3.413684000
C	-1.424383000	2.603057000	1.068348000
O	-1.834345000	2.078464000	2.243355000
H	-0.343728000	2.829949000	1.018080000
C	-2.146756000	3.881722000	0.765128000
C	-3.256437000	4.438172000	1.311882000
O	-1.647726000	4.706822000	-0.193884000
C	-3.463437000	5.677760000	0.637386000
H	-3.833812000	3.994678000	2.105476000
C	-2.458899000	5.785826000	-0.264653000
H	-4.251567000	6.396631000	0.802343000
H	-2.190027000	6.535112000	-0.991267000
H	-0.613990000	1.829626000	3.162847000
O	0.215555000	1.745234000	3.743803000
C	0.215807000	2.799370000	4.650363000
H	0.178788000	3.784697000	4.159778000
H	-0.631773000	2.756547000	5.353468000
H	1.137410000	2.759531000	5.243851000

IMes-V-B

Etot = -1724.801682514534 a.u.

C	0.455327000	-1.749392000	-0.202276000
C	-0.781509000	0.193833000	-0.227487000
C	0.522885000	0.527943000	-0.094986000
H	0.988467000	1.496939000	-0.022176000
N	-0.787715000	-1.199729000	-0.286434000
N	1.247320000	-0.653078000	-0.088632000
C	2.658416000	-0.720154000	0.048965000
C	3.439875000	-1.053008000	-1.059506000
C	3.239172000	-0.456733000	1.290257000
C	4.819773000	-1.103841000	-0.903035000
C	4.625023000	-0.514803000	1.397835000
C	5.432588000	-0.831177000	0.314013000
H	5.432403000	-1.366696000	-1.761171000
H	5.081906000	-0.319860000	2.364238000
C	-1.923000000	-2.071209000	-0.371279000
C	-2.451924000	-2.395010000	-1.617635000
C	-2.411701000	-2.645871000	0.798853000
C	-3.503445000	-3.300057000	-1.670162000
C	-3.464575000	-3.547204000	0.698254000
C	-4.029090000	-3.882029000	-0.524903000
H	-3.934436000	-3.540028000	-2.637962000
H	-3.857235000	-3.994282000	1.607795000
C	-1.828536000	-2.293890000	2.131346000
H	-0.767077000	-2.555136000	2.168427000
H	-1.910744000	-1.220099000	2.323577000
H	-2.347106000	-2.828063000	2.929861000
C	-1.930501000	-1.760550000	-2.866717000
H	-2.212442000	-0.704593000	-2.906121000
H	-0.839850000	-1.813701000	-2.913571000
H	-2.344398000	-2.251787000	-3.748843000
C	2.805266000	-1.361398000	-2.379359000
H	2.160330000	-2.239247000	-2.296656000
H	2.166965000	-0.539219000	-2.713603000
H	3.565789000	-1.542423000	-3.140800000
C	2.392756000	-0.152352000	2.487842000
H	1.923820000	0.832351000	2.415507000
H	1.579839000	-0.875448000	2.583358000
H	2.993570000	-0.174997000	3.398366000
C	6.926657000	-0.859996000	0.446383000
H	7.368960000	0.093433000	0.138887000
H	7.230228000	-1.042754000	1.479243000
H	7.367053000	-1.638854000	-0.180345000
C	-5.199028000	-4.817514000	-0.607258000
H	-5.280001000	-5.433171000	0.291511000
H	-6.136586000	-4.261958000	-0.713507000

H	-5.118411000	-5.484260000	-1.469815000
C	-2.015308000	1.094227000	-0.297089000
O	-3.162521000	0.394804000	-0.223923000
H	-3.214156000	0.708042000	1.324945000
C	-1.912889000	1.931861000	-1.551881000
C	-0.960971000	2.117070000	-2.507952000
O	-3.005112000	2.667523000	-1.866299000
C	-1.507388000	3.026903000	-3.461142000
H	0.008182000	1.648256000	-2.532177000
C	-2.750069000	3.322436000	-3.014710000
H	-1.041808000	3.399299000	-4.360501000
H	-3.545391000	3.945072000	-3.390071000
C	-1.966618000	2.022869000	1.047973000
O	-2.697986000	1.294085000	1.974985000
H	-0.919330000	2.121559000	1.357725000
C	-2.536831000	3.388519000	0.901082000
C	-3.738538000	3.922715000	1.235172000
O	-1.751027000	4.342841000	0.337551000
C	-3.696137000	5.291228000	0.835806000
H	-4.546037000	3.384547000	1.702183000
C	-2.469910000	5.487636000	0.296467000
H	-4.474584000	6.031933000	0.936410000
H	-1.976615000	6.342383000	-0.136216000
O	-5.075936000	0.117957000	-2.031548000
C	-6.081419000	1.010031000	-1.671578000
H	-6.535852000	0.769593000	-0.696598000
H	-5.726741000	2.049900000	-1.618770000
H	-6.877285000	0.964036000	-2.424639000
H	-4.332080000	0.219749000	-1.378630000

VI...IMes-I(H)-B

Etot = -1724.783763755919 a.u.

C	0.355389000	-2.325204000	0.527644000
C	-0.825993000	-0.395656000	0.092008000
C	0.396406000	-0.253661000	-0.452956000
H	0.819647000	0.566486000	-1.007927000
N	-0.823602000	-1.660105000	0.672933000
N	1.094090000	-1.426477000	-0.176479000
C	2.429995000	-1.670947000	-0.587454000
C	2.731674000	-1.729530000	-1.949981000
C	3.427002000	-1.841458000	0.378810000
C	4.050778000	-1.963962000	-2.326946000
C	4.727613000	-2.078977000	-0.048113000
C	5.062808000	-2.140134000	-1.395186000
H	4.285848000	-2.019485000	-3.386423000
H	5.503386000	-2.214692000	0.700782000

C	-1.937949000	-2.211926000	1.365663000
C	-2.524998000	-3.387870000	0.888891000
C	-2.430963000	-1.565514000	2.502211000
C	-3.604730000	-3.918084000	1.584394000
C	-3.517125000	-2.136679000	3.159735000
C	-4.117646000	-3.306788000	2.721412000
H	-4.062128000	-4.832989000	1.216894000
H	-3.901756000	-1.639974000	4.046210000
C	-1.841351000	-0.287152000	3.006421000
H	-0.751191000	-0.297324000	2.938998000
H	-2.205298000	0.561882000	2.408686000
H	-2.125819000	-0.128521000	4.049123000
C	-2.028545000	-4.065822000	-0.351303000
H	-1.982241000	-3.363623000	-1.188193000
H	-1.015256000	-4.446697000	-0.210216000
H	-2.692230000	-4.888400000	-0.625855000
C	1.672328000	-1.559200000	-2.995787000
H	0.751776000	-2.073057000	-2.712721000
H	1.417456000	-0.505074000	-3.140082000
H	2.017405000	-1.956384000	-3.952362000
C	3.113572000	-1.764376000	1.840602000
H	2.592597000	-0.833754000	2.080690000
H	2.444034000	-2.574721000	2.135588000
H	4.030377000	-1.813531000	2.431366000
C	6.482405000	-2.362623000	-1.826707000
H	7.046101000	-1.423697000	-1.831357000
H	7.001172000	-3.048974000	-1.153174000
H	6.529954000	-2.776526000	-2.836177000
C	-5.310629000	-3.876042000	3.431356000
H	-5.323798000	-3.581874000	4.483175000
H	-6.243965000	-3.520483000	2.981934000
H	-5.321135000	-4.967741000	3.383018000
C	-2.239878000	3.220921000	-0.924895000
O	-1.463134000	2.437517000	-1.435430000
H	-1.663906000	0.307808000	0.148965000
C	-2.186271000	4.643021000	-1.304431000
C	-2.786031000	5.772131000	-0.827183000
O	-1.360191000	4.977583000	-2.334378000
C	-2.304565000	6.853163000	-1.609465000
H	-3.494420000	5.809288000	-0.016900000
C	-1.443928000	6.302496000	-2.504790000
H	-2.557632000	7.897805000	-1.520295000
H	-0.838240000	6.718224000	-3.294033000
C	-3.262057000	2.763222000	0.157565000
O	-2.945079000	1.626885000	0.738692000
H	-3.331867000	3.653581000	0.843583000

C	-4.617148000	2.697940000	-0.539880000
C	-5.376150000	1.614837000	-0.840695000
O	-5.271723000	3.833441000	-0.914794000
C	-6.570967000	2.110601000	-1.442934000
H	-5.092342000	0.599207000	-0.621512000
C	-6.453368000	3.459294000	-1.462010000
H	-7.410657000	1.539721000	-1.809451000
H	-7.091930000	4.256318000	-1.807428000
O	0.554612000	2.206107000	-3.338190000
C	-0.168990000	1.821084000	-4.473534000
H	-0.824312000	0.961160000	-4.281293000
H	-0.791501000	2.636668000	-4.868477000
H	0.546075000	1.536958000	-5.250831000
H	-0.095144000	2.416363000	-2.642272000

IMes-I-C

Etot = -923.388067910936 a.u.

C	-0.012801000	-0.000113000	-0.145081000
C	0.649546000	0.001218000	1.943210000
H	1.395725000	0.001753000	2.723172000
C	-0.722163000	0.001165000	2.023244000
N	1.071505000	0.000430000	0.616248000
N	-1.074167000	0.000295000	0.662452000
C	-2.419732000	-0.000124000	0.178474000
C	-3.060763000	1.219546000	-0.038286000
C	-3.060480000	-1.220303000	-0.037021000
C	-4.377957000	1.193527000	-0.485123000
C	-4.377560000	-1.195159000	-0.483869000
C	-5.051870000	-0.000983000	-0.716752000
H	-4.890922000	2.136154000	-0.651814000
H	-4.890207000	-2.138143000	-0.649575000
C	2.421687000	0.000214000	0.145510000
C	3.063335000	-1.221703000	-0.059152000
C	3.063187000	1.222095000	-0.060777000
C	4.386142000	-1.194919000	-0.487452000
C	4.385858000	1.195027000	-0.489009000
C	5.062659000	-0.000090000	-0.710350000
H	4.901371000	-2.137299000	-0.647133000
H	4.900868000	2.137330000	-0.649924000
C	2.356686000	2.523268000	0.166938000
H	1.512208000	2.641237000	-0.517926000
H	1.956199000	2.588483000	1.181661000
H	3.038698000	3.359154000	0.011727000
C	2.357172000	-2.522772000	0.170202000
H	1.956494000	-2.586732000	1.184927000
H	1.512876000	-2.641928000	-0.514682000

H	3.039462000	-3.358668000	0.016271000
C	-2.360492000	2.520439000	0.208769000
H	-1.980046000	2.574162000	1.231933000
H	-1.501326000	2.643681000	-0.456821000
H	-3.039323000	3.357543000	0.045050000
C	-2.359765000	-2.520686000	0.211457000
H	-1.500386000	-2.644235000	-0.453799000
H	-1.979547000	-2.573267000	1.234766000
H	-3.038239000	-3.358205000	0.048392000
C	-6.461625000	-0.001688000	-1.226693000
H	-6.476932000	-0.015439000	-2.321248000
H	-7.007274000	-0.882143000	-0.882427000
H	-7.000215000	0.891212000	-0.904281000
C	6.479152000	0.000018000	-1.199925000
H	6.508424000	0.014956000	-2.294141000
H	7.020212000	0.879949000	-0.847491000
H	7.012134000	-0.893831000	-0.871273000
H	-0.019947000	-0.000786000	-1.223851000

IMes-I(H)-C Etot = -1039.045413951593 a.u.

C	-0.263489000	-0.523897000	0.202846000
C	-0.724630000	1.375613000	-0.784706000
H	-1.386193000	2.136645000	-1.167139000
C	0.646813000	1.314883000	-0.779525000
H	2.042221000	2.546563000	-0.970963000
N	-1.272017000	0.247804000	-0.182080000
N	0.870559000	0.088669000	-0.144235000
C	2.161736000	-0.478834000	0.096795000
C	2.958838000	0.055682000	1.110540000
C	2.592089000	-1.534833000	-0.703502000
C	4.203555000	-0.521710000	1.323057000
C	3.848611000	-2.074944000	-0.451191000
C	4.666992000	-1.584977000	0.556630000
H	4.834236000	-0.118395000	2.109645000
H	4.198941000	-2.894233000	-1.071652000
C	-2.658842000	-0.035014000	0.008186000
C	-3.363652000	-0.670505000	-1.015428000
C	-3.274143000	0.370860000	1.191720000
C	-4.718603000	-0.903812000	-0.820637000
C	-4.632737000	0.113822000	1.336811000
C	-5.370424000	-0.523396000	0.347330000
H	-5.282075000	-1.392370000	-1.609715000
H	-5.128209000	0.430024000	2.249565000
C	-2.502374000	1.056894000	2.277175000
H	-1.852974000	0.353447000	2.806707000

H	-1.861287000	1.846591000	1.880235000
H	-3.179461000	1.496881000	3.009370000
C	-2.684439000	-1.092112000	-2.282349000
H	-2.129558000	-0.268032000	-2.735814000
H	-1.964475000	-1.894964000	-2.099377000
H	-3.414017000	-1.456030000	-3.005653000
C	2.514952000	1.231004000	1.922583000
H	2.571098000	2.144151000	1.321872000
H	1.481128000	1.126875000	2.260167000
H	3.153314000	1.351534000	2.798657000
C	1.749481000	-2.065190000	-1.824589000
H	0.926823000	-2.687820000	-1.459287000
H	1.310686000	-1.251878000	-2.406664000
H	2.351694000	-2.680621000	-2.493516000
C	6.029184000	-2.162332000	0.797535000
H	6.195602000	-2.357488000	1.859581000
H	6.166910000	-3.098207000	0.254121000
H	6.809459000	-1.469040000	0.470216000
C	-6.828840000	-0.810372000	0.537777000
H	-6.980441000	-1.836721000	0.885911000
H	-7.272572000	-0.143580000	1.278479000
H	-7.381432000	-0.699950000	-0.397177000
H	-0.360322000	-1.472046000	0.706079000
O	2.778030000	3.216220000	-0.901694000
C	2.334258000	4.411513000	-1.467808000
H	3.114213000	5.167874000	-1.340701000
H	2.133194000	4.321102000	-2.546151000
H	1.419323000	4.796309000	-0.991212000

IMes-TS1-C $i154\text{ cm}^{-1}$ Etot = -1382.142528251881 a.u.

C	-1.806625000	-1.696368000	-0.263869000
C	-2.419255000	-0.188333000	-1.730437000
H	-3.130600000	0.419660000	-2.266600000
C	-1.051991000	-0.224368000	-1.806929000
H	2.424125000	1.752849000	-0.491914000
N	-2.872040000	-1.095567000	-0.780333000
N	-0.724624000	-1.192597000	-0.858623000
C	0.609249000	-1.618747000	-0.555138000
C	1.272349000	-1.042613000	0.527864000
C	1.207361000	-2.572203000	-1.375059000
C	2.575192000	-1.451719000	0.775891000
C	2.511685000	-2.951964000	-1.080161000
C	3.211744000	-2.400654000	-0.014907000
H	3.118392000	-0.982673000	1.589100000
H	2.996317000	-3.690080000	-1.712061000

C	-4.228999000	-1.335752000	-0.402494000
C	-4.947550000	-2.332256000	-1.061961000
C	-4.801411000	-0.536690000	0.588143000
C	-6.273993000	-2.524850000	-0.694515000
C	-6.130443000	-0.770141000	0.917958000
C	-6.881434000	-1.759387000	0.293248000
H	-6.849468000	-3.292732000	-1.202260000
H	-6.592771000	-0.154594000	1.683468000
C	-4.013129000	0.534659000	1.277029000
H	-3.210843000	0.109210000	1.886514000
H	-3.539224000	1.211640000	0.562935000
H	-4.655780000	1.121156000	1.933324000
C	-4.315906000	-3.172627000	-2.129377000
H	-3.782910000	-2.561748000	-2.860977000
H	-3.588335000	-3.871518000	-1.706391000
H	-5.071458000	-3.757879000	-2.653454000
C	0.621468000	0.005245000	1.376441000
H	0.227553000	0.814222000	0.757276000
H	-0.205715000	-0.407312000	1.963304000
H	1.347413000	0.434434000	2.065716000
C	0.479510000	-3.161819000	-2.544281000
H	-0.404654000	-3.723585000	-2.227705000
H	0.132848000	-2.381085000	-3.225497000
H	1.128129000	-3.842783000	-3.095769000
C	4.632507000	-2.787943000	0.262567000
H	4.760341000	-3.112680000	1.298270000
H	4.960412000	-3.598203000	-0.390223000
H	5.300061000	-1.936092000	0.106426000
C	-8.305314000	-2.005479000	0.690054000
H	-8.357679000	-2.692984000	1.539917000
H	-8.800700000	-1.080170000	0.989392000
H	-8.875344000	-2.450841000	-0.126777000
H	-1.827389000	-2.456669000	0.500113000
O	3.258009000	1.773128000	0.013839000
C	3.644803000	3.112999000	0.148305000
H	4.567638000	3.141295000	0.733243000
H	3.845927000	3.591828000	-0.820018000
H	2.892376000	3.717876000	0.672400000
C	0.364737000	1.569093000	-2.361644000
H	0.919319000	0.867924000	-2.999924000
O	0.818311000	1.984970000	-1.298418000
C	-0.700591000	2.277917000	-3.081973000
C	-1.100915000	2.227870000	-4.382440000
O	-1.421803000	3.207674000	-2.414754000
C	-2.140688000	3.187779000	-4.519593000
H	-0.699435000	1.577134000	-5.143084000

C	-2.289350000	3.746784000	-3.292517000
H	-2.697359000	3.436560000	-5.409096000
H	-2.937721000	4.516274000	-2.906585000

IMes-II-C Etot = -1382.186680032077 a.u.

C	-1.834440000	-1.615175000	-0.188179000
C	-2.501368000	0.121703000	-1.351576000
H	-3.202258000	0.821791000	-1.769741000
C	-1.139312000	0.111459000	-1.392552000
H	1.796257000	1.807239000	-0.548390000
N	-2.912813000	-0.953942000	-0.592099000
N	-0.755031000	-0.999198000	-0.660154000
C	0.589137000	-1.453473000	-0.427889000
C	1.244628000	-1.037502000	0.729783000
C	1.176823000	-2.287881000	-1.375891000
C	2.541976000	-1.492806000	0.918004000
C	2.476340000	-2.713457000	-1.134833000
C	3.175427000	-2.319789000	-0.000256000
H	3.082978000	-1.159618000	1.797182000
H	2.958667000	-3.358235000	-1.862785000
C	-4.266855000	-1.282447000	-0.261956000
C	-4.968834000	-2.155505000	-1.092444000
C	-4.839504000	-0.688813000	0.862104000
C	-6.287412000	-2.436577000	-0.759744000
C	-6.162294000	-1.005049000	1.148515000
C	-6.900047000	-1.875352000	0.355401000
H	-6.853755000	-3.108621000	-1.396856000
H	-6.629470000	-0.549769000	2.015938000
C	-4.064730000	0.250618000	1.734507000
H	-3.262391000	-0.269116000	2.265943000
H	-3.593985000	1.050844000	1.159320000
H	-4.716817000	0.704256000	2.480229000
C	-4.331486000	-2.769614000	-2.301342000
H	-3.870379000	-2.015232000	-2.942858000
H	-3.545774000	-3.478109000	-2.023641000
H	-5.071642000	-3.310765000	-2.890115000
C	0.595114000	-0.106855000	1.702201000
H	0.279400000	0.799880000	1.171228000
H	-0.282021000	-0.562264000	2.174667000
H	1.296065000	0.168655000	2.489236000
C	0.451499000	-2.700491000	-2.620704000
H	-0.488719000	-3.213384000	-2.397510000
H	0.206179000	-1.836038000	-3.244092000
H	1.067014000	-3.377198000	-3.213208000
C	4.598044000	-2.738209000	0.210436000

H	4.782329000	-3.014889000	1.250621000
H	4.865118000	-3.585237000	-0.423305000
H	5.274396000	-1.912985000	-0.031018000
C	-8.317008000	-2.216808000	0.701551000
H	-8.362395000	-3.154758000	1.263315000
H	-8.774192000	-1.442055000	1.318403000
H	-8.925544000	-2.345428000	-0.195353000
H	-1.833333000	-2.505901000	0.416968000
O	2.793160000	1.723685000	-0.425035000
C	3.377120000	2.946227000	-0.750136000
H	4.465088000	2.853727000	-0.660396000
H	3.156040000	3.264077000	-1.780787000
H	3.058466000	3.762151000	-0.082970000
C	-0.123562000	1.143546000	-1.848901000
H	0.710714000	0.567593000	-2.317572000
O	0.234021000	1.851264000	-0.764802000
C	-0.680124000	1.954529000	-2.989375000
C	-0.236241000	2.172388000	-4.253337000
O	-1.796702000	2.696621000	-2.768106000
C	-1.132829000	3.109726000	-4.848520000
H	0.643301000	1.732362000	-4.696293000
C	-2.055457000	3.390280000	-3.900700000
H	-1.088355000	3.527271000	-5.841967000
H	-2.913891000	4.041134000	-3.873180000

IMes-TS2-C $i438 \text{ cm}^{-1}$ $E_{\text{tot}} = -1382.151149050252 \text{ a.u.}$

C	-0.431304000	-0.816818000	0.582302000
C	0.745788000	-1.062732000	-0.078699000
N	-1.470383000	-1.157267000	-0.252531000
C	-0.964072000	-1.589064000	-1.397215000
N	0.367457000	-1.548207000	-1.327412000
H	-0.599877000	-0.447719000	1.577078000
O	3.396336000	-3.180106000	0.162524000
C	2.136803000	-0.995896000	0.391471000
O	3.047766000	-0.698195000	-0.637602000
H	3.564009000	-1.540673000	-0.662372000
C	4.290517000	-3.555651000	1.142039000
H	5.333457000	-3.582631000	0.776236000
H	4.293574000	-2.873881000	2.015031000
H	4.078498000	-4.563911000	1.544638000
H	2.516882000	-2.145859000	0.607207000
C	2.349179000	-0.113370000	1.556575000
C	3.292007000	0.830325000	1.809191000
O	1.550071000	-0.270223000	2.646872000
C	3.060729000	1.282757000	3.143374000

H	4.060131000	1.141566000	1.121828000
C	1.997407000	0.588292000	3.602683000
H	3.618664000	2.027514000	3.688865000
H	1.458645000	0.579634000	4.535292000
C	-2.864513000	-1.061731000	0.060205000
C	-3.558342000	0.088034000	-0.311581000
C	-3.469580000	-2.119664000	0.739220000
C	-4.907871000	0.156632000	0.014116000
C	-4.819933000	-1.998833000	1.039336000
C	-5.554657000	-0.871278000	0.688775000
H	-5.466713000	1.043774000	-0.266563000
H	-5.311008000	-2.812340000	1.563967000
C	1.168036000	-1.954112000	-2.456648000
C	1.540354000	-0.982257000	-3.385689000
C	1.471740000	-3.303680000	-2.611027000
C	2.237887000	-1.401285000	-4.507744000
C	2.173476000	-3.666783000	-3.757773000
C	2.565593000	-2.738844000	-4.710180000
H	2.540537000	-0.659803000	-5.240742000
H	2.426564000	-4.712979000	-3.896566000
C	1.249367000	0.467030000	-3.158173000
H	0.191908000	0.651161000	-2.948017000
H	1.825555000	0.825655000	-2.300839000
H	1.525332000	1.056295000	-4.032703000
C	1.138523000	-4.323339000	-1.571799000
H	1.867991000	-4.221071000	-0.751111000
H	0.133175000	-4.194559000	-1.162499000
H	1.209965000	-5.329149000	-1.987080000
C	3.351358000	-3.156859000	-5.915727000
H	3.038711000	-2.607273000	-6.806168000
H	4.417419000	-2.958871000	-5.768688000
H	3.239480000	-4.223820000	-6.113749000
C	-2.886717000	1.210376000	-1.042652000
H	-1.931452000	1.477886000	-0.586069000
H	-2.683646000	0.943346000	-2.083931000
H	-3.521693000	2.095992000	-1.048450000
C	-2.699842000	-3.344728000	1.126637000
H	-2.305345000	-3.865201000	0.249730000
H	-1.844249000	-3.101225000	1.760863000
H	-3.337785000	-4.040983000	1.670017000
C	-7.002078000	-0.757280000	1.057771000
H	-7.501268000	-1.726832000	1.014227000
H	-7.111180000	-0.380187000	2.079169000
H	-7.529456000	-0.069103000	0.395768000
H	-1.528181000	-1.917812000	-2.253086000

IMes-III-C Etot = -1382.162867539127 a.u.

C	-1.822071000	-1.502904000	-0.198091000
C	-2.610288000	0.207494000	-1.352745000
H	-3.369730000	0.835295000	-1.775595000
C	-1.201019000	0.307828000	-1.424274000
H	1.445145000	0.721610000	-2.542651000
N	-2.920257000	-0.897410000	-0.607713000
N	-0.753925000	-0.807844000	-0.666040000
C	0.573549000	-1.290732000	-0.483287000
C	1.383789000	-0.726695000	0.504181000
C	1.019986000	-2.339818000	-1.286790000
C	2.660911000	-1.243478000	0.676157000
C	2.309116000	-2.826040000	-1.077082000
C	3.142504000	-2.293926000	-0.098638000
H	3.301020000	-0.807595000	1.437295000
H	2.667124000	-3.643238000	-1.696695000
C	-4.249062000	-1.313420000	-0.285055000
C	-4.926337000	-2.149078000	-1.173355000
C	-4.830803000	-0.846191000	0.891412000
C	-6.223053000	-2.522519000	-0.845062000
C	-6.131198000	-1.251269000	1.173382000
C	-6.840754000	-2.088842000	0.323093000
H	-6.768582000	-3.165874000	-1.528715000
H	-6.603873000	-0.889849000	2.081467000
C	-4.089247000	0.054874000	1.831377000
H	-3.431312000	-0.519887000	2.489960000
H	-3.468721000	0.773842000	1.293619000
H	-4.787132000	0.605122000	2.463145000
C	-4.281859000	-2.639638000	-2.433720000
H	-3.747101000	-1.839988000	-2.949614000
H	-3.555967000	-3.429996000	-2.221322000
H	-5.030360000	-3.050225000	-3.111533000
C	0.900879000	0.428827000	1.318189000
H	0.788100000	1.307614000	0.677796000
H	-0.074899000	0.225076000	1.765613000
H	1.605244000	0.664430000	2.116364000
C	0.155861000	-2.907736000	-2.370857000
H	-0.706950000	-3.439595000	-1.959147000
H	-0.233633000	-2.118290000	-3.017850000
H	0.720682000	-3.608909000	-2.985490000
C	4.512180000	-2.855950000	0.136518000
H	4.500644000	-3.573171000	0.963057000
H	4.886241000	-3.379409000	-0.744970000
H	5.225551000	-2.072120000	0.398672000
C	-8.233847000	-2.527461000	0.659096000
H	-8.229680000	-3.526407000	1.105869000

H	-8.703333000	-1.849632000	1.373395000
H	-8.861962000	-2.573734000	-0.232673000
H	-1.776309000	-2.373845000	0.430038000
O	2.824037000	-0.383329000	-3.312563000
C	4.030081000	0.354056000	-3.313948000
H	4.898935000	-0.291001000	-3.485672000
H	3.967020000	1.070835000	-4.132609000
H	4.172838000	0.906793000	-2.379138000
C	-0.381562000	1.221869000	-2.055478000
O	0.986778000	1.193434000	-1.828542000
C	-0.848813000	2.304311000	-2.849526000
C	-0.174768000	3.325729000	-3.477695000
O	-2.184827000	2.428561000	-3.098589000
C	-1.160405000	4.106844000	-4.142958000
H	0.888954000	3.489362000	-3.444891000
C	-2.356385000	3.531378000	-3.887688000
H	-0.999111000	4.992866000	-4.737702000
H	-3.371174000	3.758898000	-4.166102000
H	2.850999000	-1.026668000	-2.594005000

IMes-IV-C Etot = -1725.305968840181 a.u.

C	0.546636000	-1.318228000	0.077691000
C	-0.552775000	0.584556000	-0.165186000
C	0.774145000	0.852051000	-0.015865000
H	1.292915000	1.791956000	0.041192000
N	-0.663414000	-0.797062000	-0.102215000
N	1.440043000	-0.339825000	0.130106000
C	2.852051000	-0.506076000	0.317531000
C	3.691118000	-0.331360000	-0.784197000
C	3.329948000	-0.826858000	1.588130000
C	5.055601000	-0.486647000	-0.583359000
C	4.706693000	-0.969038000	1.728455000
C	5.582870000	-0.800120000	0.664665000
H	5.724335000	-0.361674000	-1.429227000
H	5.102103000	-1.215902000	2.708536000
C	-1.827639000	-1.646627000	-0.179125000
C	-2.269305000	-2.061277000	-1.431025000
C	-2.416557000	-2.067736000	1.011537000
C	-3.357421000	-2.924716000	-1.470793000
C	-3.499415000	-2.930810000	0.911815000
C	-3.988810000	-3.364485000	-0.314922000
H	-3.721687000	-3.257506000	-2.437654000
H	-3.980718000	-3.264937000	1.825604000
C	-1.929229000	-1.590801000	2.343398000
H	-0.910126000	-1.928857000	2.552860000

H	-1.913538000	-0.498753000	2.400780000
H	-2.571291000	-1.968505000	3.138890000
C	-1.619410000	-1.591175000	-2.694882000
H	-1.725246000	-0.509774000	-2.818357000
H	-0.548263000	-1.814327000	-2.709988000
H	-2.071972000	-2.076996000	-3.559142000
C	3.156780000	0.013696000	-2.141272000
H	2.294794000	-0.600679000	-2.411186000
H	2.834678000	1.057669000	-2.191241000
H	3.926027000	-0.129596000	-2.899839000
C	2.417974000	-1.013973000	2.760289000
H	1.668331000	-0.218568000	2.844288000
H	1.880936000	-1.965984000	2.694270000
H	2.997941000	-1.039121000	3.683149000
C	7.062774000	-0.927795000	0.858492000
H	7.519550000	0.056490000	0.999328000
H	7.299146000	-1.528434000	1.737731000
H	7.540008000	-1.386080000	-0.009750000
C	-5.187847000	-4.259953000	-0.387677000
H	-5.233121000	-4.936385000	0.467746000
H	-6.109185000	-3.669506000	-0.386143000
H	-5.184198000	-4.858933000	-1.299861000
C	-1.717496000	1.541802000	-0.294865000
O	-2.901185000	0.908342000	0.048805000
H	-2.915676000	1.140723000	1.029879000
C	-1.774170000	2.082329000	-1.683974000
C	-0.858595000	2.199781000	-2.685339000
O	-2.939076000	2.644839000	-2.066377000
C	-1.510213000	2.891856000	-3.747925000
H	0.157219000	1.839764000	-2.670401000
C	-2.767825000	3.133826000	-3.311648000
H	-1.097835000	3.166620000	-4.705627000
H	-3.625937000	3.614428000	-3.750970000
C	-1.505150000	2.647717000	0.875382000
O	-1.932759000	2.041132000	2.001835000
H	-0.426764000	2.899271000	0.869549000
C	-2.248234000	3.912704000	0.591532000
C	-3.399019000	4.420733000	1.094919000
O	-1.716394000	4.777920000	-0.311366000
C	-3.598506000	5.678275000	0.451928000
H	-4.011211000	3.943618000	1.841675000
C	-2.550483000	5.840114000	-0.389163000
H	-4.410365000	6.372865000	0.600688000
H	-2.259424000	6.623052000	-1.069940000
H	-0.684678000	1.590546000	2.794583000
O	0.177689000	1.310313000	3.252653000

C	0.324859000	2.062783000	4.421201000
H	0.350039000	3.143571000	4.224158000
H	-0.482404000	1.877140000	5.143723000
H	1.270434000	1.790542000	4.902470000
H	0.760261000	-2.369901000	0.163333000

IMes-V-C Etot = -1725.305416199688 a.u.

C	0.389567000	-1.600905000	-0.148060000
C	-0.773166000	0.276638000	-0.239028000
C	0.552835000	0.577359000	-0.131708000
H	1.049539000	1.531297000	-0.092866000
N	-0.840501000	-1.105738000	-0.243575000
N	1.259962000	-0.601143000	-0.079357000
C	2.681148000	-0.736939000	0.042151000
C	3.435473000	-0.953879000	-1.110361000
C	3.254139000	-0.637052000	1.309818000
C	4.811337000	-1.075539000	-0.962138000
C	4.634341000	-0.766930000	1.399647000
C	5.428830000	-0.983192000	0.279771000
H	5.417035000	-1.245427000	-1.846673000
H	5.100230000	-0.698210000	2.377454000
C	-1.974967000	-2.001666000	-0.301488000
C	-2.492646000	-2.356218000	-1.542849000
C	-2.425623000	-2.554522000	0.894916000
C	-3.514436000	-3.296656000	-1.558266000
C	-3.451198000	-3.486662000	0.819209000
C	-4.011699000	-3.866307000	-0.394607000
H	-3.948294000	-3.569814000	-2.514582000
H	-3.828457000	-3.920436000	1.740112000
C	-1.855389000	-2.146518000	2.219229000
H	-0.819193000	-2.481368000	2.339162000
H	-1.870564000	-1.060224000	2.343601000
H	-2.432780000	-2.589463000	3.030775000
C	-2.038058000	-1.714542000	-2.814039000
H	-2.570769000	-0.769575000	-2.956721000
H	-0.966177000	-1.504223000	-2.821775000
H	-2.266526000	-2.354527000	-3.666907000
C	2.797496000	-1.062306000	-2.461854000
H	2.257496000	-2.006561000	-2.576929000
H	2.079321000	-0.258789000	-2.638955000
H	3.554018000	-1.019165000	-3.244867000
C	2.422252000	-0.403546000	2.533388000
H	1.921460000	0.567352000	2.503605000
H	1.638723000	-1.157732000	2.640958000
H	3.043249000	-0.432729000	3.428037000

C	6.917940000	-1.086535000	0.403897000
H	7.385993000	-0.109360000	0.250954000
H	7.211680000	-1.438929000	1.393622000
H	7.333506000	-1.767044000	-0.341084000
C	-5.151176000	-4.837862000	-0.446031000
H	-5.198467000	-5.447463000	0.457828000
H	-6.103164000	-4.306369000	-0.537885000
H	-5.068175000	-5.505010000	-1.306444000
C	-2.003429000	1.183936000	-0.288786000
O	-3.129362000	0.468622000	-0.175221000
H	-3.096919000	0.778834000	1.440113000
C	-1.911307000	2.004049000	-1.554996000
C	-0.959766000	2.205993000	-2.507807000
O	-3.015430000	2.713171000	-1.869617000
C	-1.522199000	3.103979000	-3.462617000
H	0.022942000	1.765597000	-2.540731000
C	-2.770856000	3.372978000	-3.018914000
H	-1.061553000	3.486593000	-4.359426000
H	-3.577237000	3.979977000	-3.395315000
C	-1.894057000	2.109931000	1.042319000
O	-2.501321000	1.338225000	2.025240000
H	-0.835266000	2.274469000	1.279718000
C	-2.549400000	3.437882000	0.923610000
C	-3.764319000	3.903459000	1.302452000
O	-1.837525000	4.427770000	0.326906000
C	-3.811327000	5.270870000	0.899903000
H	-4.525196000	3.330311000	1.805052000
C	-2.620144000	5.531557000	0.313323000
H	-4.623277000	5.968169000	1.033784000
H	-2.189791000	6.412148000	-0.133901000
O	-4.805388000	-0.049927000	-2.174021000
C	-5.956613000	0.735948000	-2.089330000
H	-6.545026000	0.524335000	-1.184199000
H	-5.733318000	1.811789000	-2.095957000
H	-6.589620000	0.517805000	-2.954848000
H	-4.209256000	0.180019000	-1.417381000
H	0.633108000	-2.649477000	-0.122722000

VI...IMes-I(H)-C

Etot = -1725.287948318512 a.u.

C	0.240456000	-2.162864000	0.456821000
C	-0.854693000	-0.264159000	0.116905000
C	0.356833000	-0.184574000	-0.493564000
H	0.791478000	0.602713000	-1.091070000
N	-0.896840000	-1.515123000	0.701110000
N	1.023169000	-1.372562000	-0.272286000

C	2.336155000	-1.702530000	-0.735744000
C	2.534792000	-1.881421000	-2.106696000
C	3.372195000	-1.808053000	0.191428000
C	3.818539000	-2.200321000	-2.529392000
C	4.636678000	-2.128769000	-0.288967000
C	4.880199000	-2.329412000	-1.641093000
H	3.991131000	-2.351895000	-3.590397000
H	5.455894000	-2.213326000	0.418163000
C	-2.001683000	-2.059100000	1.435006000
C	-2.672865000	-3.165245000	0.914537000
C	-2.382014000	-1.441891000	2.628853000
C	-3.735946000	-3.678920000	1.647839000
C	-3.450159000	-2.001078000	3.318802000
C	-4.137445000	-3.113848000	2.850837000
H	-4.273914000	-4.536071000	1.254967000
H	-3.759553000	-1.537477000	4.250206000
C	-1.714675000	-0.205381000	3.136006000
H	-0.625724000	-0.266367000	3.062108000
H	-2.046239000	0.658404000	2.540175000
H	-1.977571000	-0.036257000	4.180733000
C	-2.308566000	-3.780778000	-0.404682000
H	-2.074803000	-3.020913000	-1.153569000
H	-1.443694000	-4.446767000	-0.328526000
H	-3.140220000	-4.377171000	-0.780402000
C	1.423075000	-1.721773000	-3.097003000
H	0.508665000	-2.219539000	-2.766150000
H	1.178190000	-0.665391000	-3.248846000
H	1.711726000	-2.143954000	-4.059729000
C	3.158248000	-1.573746000	1.657043000
H	2.496617000	-0.724513000	1.839515000
H	2.714693000	-2.444269000	2.149174000
H	4.110053000	-1.373937000	2.149406000
C	6.258101000	-2.644785000	-2.137852000
H	6.741167000	-1.746658000	-2.534375000
H	6.890876000	-3.034406000	-1.339326000
H	6.230971000	-3.380479000	-2.944064000
C	-5.310490000	-3.660675000	3.605922000
H	-5.134353000	-3.639568000	4.683268000
H	-6.206002000	-3.062613000	3.412043000
H	-5.530011000	-4.688795000	3.314115000
C	-2.348422000	2.999550000	-1.073048000
O	-1.542762000	2.221335000	-1.553206000
H	-1.693622000	0.494904000	0.229359000
C	-2.424378000	4.373364000	-1.570905000
C	-3.126656000	5.477938000	-1.182191000
O	-1.635380000	4.694481000	-2.634751000

C	-2.752077000	6.528250000	-2.055889000
H	-3.836006000	5.519587000	-0.372814000
C	-1.846354000	5.987414000	-2.911864000
H	-3.104147000	7.547264000	-2.052482000
H	-1.288301000	6.393031000	-3.740525000
C	-3.275745000	2.564813000	0.092284000
O	-2.808595000	1.511572000	0.760129000
H	-3.393902000	3.485186000	0.714215000
C	-4.643133000	2.299793000	-0.510875000
C	-5.307349000	1.132160000	-0.693873000
O	-5.415647000	3.337929000	-0.928775000
C	-6.570570000	1.470693000	-1.265586000
H	-4.928159000	0.161942000	-0.420786000
C	-6.580791000	2.818199000	-1.385298000
H	-7.368747000	0.800643000	-1.545020000
H	-7.305769000	3.526067000	-1.752116000
O	0.788314000	1.833649000	-2.927046000
C	1.433566000	2.968149000	-3.444176000
H	0.885649000	3.404255000	-4.288752000
H	1.572424000	3.749902000	-2.686802000
H	2.419231000	2.661606000	-3.801110000
H	-0.086858000	2.096107000	-2.582342000
H	0.487929000	-3.155863000	0.789092000

[IPrH]⁺ Etot = -1159.555789437028 a.u.

C	-0.004759000	-0.002413000	-0.134173000
C	0.661983000	0.020719000	1.960596000
H	1.369087000	0.031035000	2.772744000
C	-0.692565000	0.017014000	1.953769000
H	-1.407894000	0.023511000	2.758712000
N	1.069328000	0.008754000	0.647161000
N	-1.086655000	0.001914000	0.636315000
C	-2.445382000	-0.006730000	0.162171000
C	-3.068215000	1.221167000	-0.078349000
C	-3.070601000	-1.242588000	-0.026033000
C	-4.382367000	1.182109000	-0.534901000
C	-4.384726000	-1.220397000	-0.483681000
C	-5.033425000	-0.023312000	-0.735446000
H	-4.901440000	2.112106000	-0.737173000
H	-4.905498000	-2.157125000	-0.646587000
C	2.432374000	0.007460000	0.185428000
C	3.057957000	-1.225333000	-0.020948000
C	3.058360000	1.239048000	-0.026232000
C	4.375481000	-1.195874000	-0.468296000
C	4.376058000	1.207189000	-0.473038000

C	5.027288000	0.005091000	-0.692048000
H	4.896532000	-2.129876000	-0.645296000
H	4.897432000	2.140302000	-0.653782000
C	2.365516000	2.565667000	0.194428000
H	1.369025000	2.375151000	0.599821000
C	2.364543000	-2.550583000	0.205969000
H	1.370317000	-2.357641000	0.615778000
C	-2.376473000	2.551134000	0.124818000
H	-1.380099000	2.366642000	0.533194000
C	-2.380545000	-2.564078000	0.231225000
H	-1.385056000	-2.364588000	0.634721000
H	0.000827000	-0.013898000	-1.212518000
H	-6.057368000	-0.029836000	-1.092295000
H	6.053850000	0.004179000	-1.041358000
C	-3.132445000	-3.393692000	1.269876000
H	-4.128185000	-3.667755000	0.912420000
H	-2.585526000	-4.316840000	1.476356000
H	-3.246725000	-2.846377000	2.208418000
C	-2.196958000	-3.345641000	-1.068967000
H	-1.625959000	-2.769930000	-1.801303000
H	-1.661621000	-4.278024000	-0.873223000
H	-3.162969000	-3.598274000	-1.513958000
C	-3.124614000	3.420711000	1.133146000
H	-4.121955000	3.680217000	0.769370000
H	-3.234549000	2.910407000	2.092810000
H	-2.577215000	4.351375000	1.301044000
C	-2.196277000	3.281534000	-1.205269000
H	-1.630696000	2.675996000	-1.917457000
H	-3.163388000	3.520309000	-1.655463000
H	-1.656977000	4.218935000	-1.048317000
C	3.114096000	-3.406995000	1.224411000
H	3.227788000	-2.883504000	2.176487000
H	2.564737000	-4.333769000	1.406879000
H	4.109692000	-3.674634000	0.861889000
C	2.177878000	-3.300842000	-1.112151000
H	3.143198000	-3.546029000	-1.562830000
H	1.639587000	-4.235884000	-0.938271000
H	1.608824000	-2.706501000	-1.830932000
C	3.111902000	3.423059000	1.214398000
H	3.219977000	2.901757000	2.168334000
H	4.109813000	3.687429000	0.855807000
H	2.563822000	4.351549000	1.391937000
C	2.185949000	3.313395000	-1.126120000
H	3.153574000	3.557298000	-1.572501000
H	1.620043000	2.717930000	-1.846437000
H	1.647365000	4.249087000	-0.956693000

IPr-I-A Etot = -1159.060194166290 a.u.

C	-0.005321000	-0.004520000	-0.270985000
C	0.660568000	0.019563000	1.912940000
H	1.366813000	0.029381000	2.726914000
C	-0.688759000	0.017446000	1.907536000
H	-1.401518000	0.025067000	2.715833000
N	1.048170000	0.006108000	0.586664000
N	-1.065683000	0.002739000	0.578209000
C	-2.427733000	-0.004165000	0.144638000
C	-3.072344000	1.218764000	-0.075193000
C	-3.071161000	-1.233667000	-0.039054000
C	-4.398451000	1.185307000	-0.498466000
C	-4.397286000	-1.213972000	-0.463066000
C	-5.056470000	-0.017757000	-0.691545000
H	-4.922532000	2.117332000	-0.680379000
H	-4.920451000	-2.151430000	-0.617611000
C	2.413638000	0.004015000	0.163909000
C	3.060389000	-1.223252000	-0.022961000
C	3.058112000	1.229373000	-0.042298000
C	4.389842000	-1.198666000	-0.436182000
C	4.387690000	1.200806000	-0.454912000
C	5.049058000	0.000066000	-0.650984000
H	4.915594000	-2.134290000	-0.593020000
H	4.911720000	2.134847000	-0.626284000
C	2.361258000	2.557504000	0.158011000
H	1.347620000	2.357140000	0.510940000
C	2.366072000	-2.549311000	0.198613000
H	1.352831000	-2.345189000	0.550522000
C	-2.379573000	2.549347000	0.122916000
H	-1.367774000	2.352835000	0.483187000
C	-2.376894000	-2.557168000	0.197644000
H	-1.365471000	-2.349191000	0.552498000
H	-6.089473000	-0.023119000	-1.022237000
H	6.084705000	-0.001518000	-0.973340000
C	-3.084847000	-3.375244000	1.275868000
H	-4.098974000	-3.643811000	0.968078000
H	-2.536990000	-4.301938000	1.465478000
H	-3.152066000	-2.820459000	2.214855000
C	-2.251317000	-3.354626000	-1.099498000
H	-1.710670000	-2.787956000	-1.861363000
H	-1.709551000	-4.286732000	-0.918332000
H	-3.235324000	-3.610749000	-1.501677000
C	-3.087896000	3.397297000	1.177555000
H	-4.102657000	3.655326000	0.862954000
H	-3.153345000	2.869852000	2.132282000

H	-2.541223000	4.329885000	1.339712000
C	-2.255689000	3.309166000	-1.196759000
H	-1.717392000	2.720226000	-1.943237000
H	-3.240254000	3.554810000	-1.604109000
H	-1.712537000	4.245481000	-1.043641000
C	3.069026000	-3.376854000	1.272893000
H	3.131070000	-2.830618000	2.217222000
H	2.520408000	-4.305352000	1.451153000
H	4.084756000	-3.642492000	0.967942000
C	2.247664000	-3.334910000	-1.106392000
H	3.234037000	-3.587321000	-1.505163000
H	1.704802000	-4.268596000	-0.937013000
H	1.711568000	-2.761290000	-1.866263000
C	3.060795000	3.402038000	1.221234000
H	3.121419000	2.870171000	2.173820000
H	4.076878000	3.664221000	0.914459000
H	2.510693000	4.332446000	1.384302000
C	2.244257000	3.323341000	-1.158810000
H	3.231001000	3.571829000	-1.559102000
H	1.711021000	2.737406000	-1.911264000
H	1.699218000	4.258370000	-1.004516000

IPr-I(H)-A Etot = -1274.716795483306 a.u.

C	-1.814182000	0.352321000	-0.223003000
C	-2.572676000	2.063446000	-1.512235000
H	-3.298821000	2.761966000	-1.894142000
C	-1.266919000	1.888191000	-1.806354000
N	-2.879604000	1.121537000	-0.550579000
N	-0.830672000	0.846724000	-1.011772000
C	0.510727000	0.349058000	-1.019333000
C	1.460268000	0.963888000	-0.195076000
C	0.826599000	-0.726678000	-1.857108000
C	2.760630000	0.467318000	-0.225227000
C	2.139953000	-1.188858000	-1.847191000
C	3.099017000	-0.598981000	-1.041236000
H	3.518799000	0.923782000	0.401651000
H	2.414490000	-2.022981000	-2.483581000
C	-4.176753000	0.977731000	0.035718000
C	-5.077423000	0.071019000	-0.534513000
C	-4.500734000	1.759002000	1.151120000
C	-6.335015000	-0.045041000	0.051906000
C	-5.772696000	1.609334000	1.696968000
C	-6.681667000	0.715860000	1.155471000
H	-7.054103000	-0.741505000	-0.365227000
H	-6.054623000	2.202421000	2.559968000

C	-3.532979000	2.751754000	1.757890000
H	-2.572917000	2.644245000	1.248551000
C	-4.733594000	-0.766551000	-1.747070000
H	-3.713698000	-0.522064000	-2.050749000
C	1.122432000	2.133043000	0.704248000
H	0.052222000	2.331221000	0.615775000
C	-0.194843000	-1.385352000	-2.758350000
H	-1.151120000	-0.878250000	-2.614865000
H	-1.788706000	-1.130913000	0.838892000
H	-0.619995000	2.402841000	-2.497507000
O	-1.791027000	-1.951198000	1.417383000
C	-1.445640000	-1.564334000	2.724309000
H	-2.209470000	-1.889991000	3.440255000
H	-0.489182000	-2.006961000	3.030694000
H	-1.350435000	-0.475292000	2.810565000
H	4.117278000	-0.972441000	-1.049550000
H	-7.667193000	0.612378000	1.596379000
C	-0.396257000	-2.854333000	-2.391193000
H	-1.171668000	-3.297044000	-3.021998000
H	0.522751000	-3.428097000	-2.538794000
H	-0.701407000	-2.964347000	-1.347901000
C	0.188405000	-1.237318000	-4.229926000
H	1.130505000	-1.747903000	-4.446411000
H	-0.584296000	-1.675843000	-4.866679000
H	0.302474000	-0.186366000	-4.505999000
C	1.864354000	3.395148000	0.266551000
H	1.577302000	4.240284000	0.897501000
H	2.946482000	3.264550000	0.353059000
H	1.636549000	3.650056000	-0.771161000
C	1.406773000	1.813173000	2.170521000
H	0.854003000	0.929326000	2.497380000
H	2.471330000	1.629486000	2.337670000
H	1.110427000	2.654488000	2.802389000
C	-3.294471000	2.477466000	3.241232000
H	-4.208952000	2.614166000	3.824337000
H	-2.936958000	1.457879000	3.404135000
H	-2.543939000	3.168668000	3.633495000
C	-4.014157000	4.185855000	1.539796000
H	-4.142991000	4.404538000	0.477006000
H	-4.971725000	4.357403000	2.039329000
H	-3.289373000	4.894157000	1.949396000
C	-5.653802000	-0.443237000	-2.922944000
H	-5.358032000	-1.021056000	-3.802329000
H	-6.693040000	-0.692700000	-2.692730000
H	-5.609875000	0.617727000	-3.181012000
C	-4.767106000	-2.258509000	-1.419943000

H	-5.767514000	-2.573300000	-1.110922000
H	-4.489526000	-2.842998000	-2.301238000
H	-4.068798000	-2.502934000	-0.616161000

IPr-TS1-A $i149\text{ cm}^{-1}$ Etot = -1617.809969802293 a.u.

H	-1.331504000	4.078821000	0.250352000
C	-2.222391000	2.166688000	0.910371000
C	-1.356535000	3.003312000	0.305128000
N	-1.774255000	0.887120000	0.643036000
C	-0.652321000	0.891849000	-0.111764000
N	-0.407206000	2.207301000	-0.308892000
H	-3.106179000	2.360009000	1.495326000
H	2.810677000	-0.819707000	1.331568000
O	3.357627000	-1.121889000	2.087988000
C	0.788510000	-0.863224000	-0.268717000
O	1.931173000	-0.401736000	-0.117492000
C	0.666214000	2.748500000	-1.091931000
C	1.822717000	3.189097000	-0.437627000
C	0.491813000	2.868886000	-2.477324000
C	2.830772000	3.749736000	-1.217645000
C	1.532981000	3.430781000	-3.210727000
C	2.691510000	3.866086000	-2.589615000
H	3.738426000	4.102431000	-0.741873000
H	1.431886000	3.537762000	-4.284231000
C	-2.461475000	-0.291022000	1.084377000
C	-3.519602000	-0.776987000	0.306329000
C	-2.078978000	-0.885756000	2.293544000
C	-4.189044000	-1.908784000	0.764170000
C	-2.779129000	-2.016882000	2.704011000
C	-3.821267000	-2.525987000	1.947358000
H	-5.014752000	-2.309001000	0.186900000
H	-2.509331000	-2.502538000	3.634464000
C	1.982610000	3.114784000	1.065429000
H	1.227311000	2.424794000	1.449697000
C	-0.989934000	-0.303486000	3.168862000
H	-0.387151000	0.369554000	2.553933000
C	-3.979782000	-0.087795000	-0.960673000
H	-3.219987000	0.644497000	-1.242388000
C	-0.799986000	2.478640000	-3.163700000
H	-1.313677000	1.756180000	-2.524980000
H	0.218559000	-1.265678000	0.578924000
C	0.364073000	-1.453601000	-1.539868000
C	-0.524643000	-2.448499000	-1.808139000
O	1.005672000	-1.088088000	-2.676254000
C	-0.429010000	-2.705644000	-3.204937000

H	-1.161856000	-2.940126000	-1.088980000
C	0.511351000	-1.850067000	-3.676479000
H	-0.980273000	-3.432319000	-3.781194000
H	0.924000000	-1.672800000	-4.656891000
C	4.609099000	-1.527561000	1.582960000
H	5.148302000	-0.701520000	1.101886000
H	5.214008000	-1.884178000	2.419286000
H	4.516913000	-2.345152000	0.857117000
H	3.489686000	4.303477000	-3.179529000
H	-4.354665000	-3.407465000	2.286206000
C	3.348167000	2.578880000	1.485700000
H	3.376148000	2.452559000	2.570924000
H	3.554424000	1.611281000	1.025406000
H	4.151848000	3.268446000	1.215967000
C	1.734466000	4.485344000	1.698545000
H	0.745138000	4.874905000	1.449001000
H	1.810451000	4.418646000	2.787049000
H	2.478718000	5.207704000	1.351114000
C	-1.606479000	0.526175000	4.296998000
H	-2.244631000	1.322919000	3.908219000
H	-2.214514000	-0.106866000	4.949540000
H	-0.820503000	0.983149000	4.903908000
C	-0.053611000	-1.364249000	3.739322000
H	-0.567188000	-2.016864000	4.449485000
H	0.375739000	-1.988571000	2.952443000
H	0.767774000	-0.880975000	4.273600000
C	-5.284896000	0.669603000	-0.709776000
H	-5.589794000	1.206596000	-1.611780000
H	-6.087314000	-0.023142000	-0.440755000
H	-5.178940000	1.394691000	0.100420000
C	-4.138505000	-1.051656000	-2.133104000
H	-3.212415000	-1.594485000	-2.331772000
H	-4.930634000	-1.782099000	-1.950695000
H	-4.406369000	-0.494698000	-3.034556000
C	-0.584687000	1.815339000	-4.519773000
H	-0.180644000	2.516510000	-5.254160000
H	0.097301000	0.966177000	-4.448580000
H	-1.540391000	1.453493000	-4.906820000
C	-1.708486000	3.701393000	-3.312495000
H	-1.238036000	4.449743000	-3.956852000
H	-2.660466000	3.413307000	-3.766282000
H	-1.918397000	4.169405000	-2.348427000

IPr-II-A Etot -1617.840101 a.u.

C	-0.313375000	-0.416613000	0.069480000
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C	-1.165630000	-2.147880000	-1.038625000
C	0.165842000	-2.335102000	-0.942328000
N	-1.445722000	-0.956642000	-0.408781000
N	0.682918000	-1.255200000	-0.258918000
C	2.094259000	-1.106115000	-0.007290000
C	2.891226000	-0.567288000	-1.025533000
C	2.615907000	-1.592375000	1.197041000
C	4.257688000	-0.471925000	-0.779152000
C	3.989224000	-1.469207000	1.388285000
C	4.800385000	-0.908146000	0.417053000
H	4.907166000	-0.054335000	-1.539009000
H	4.431640000	-1.828343000	2.309642000
C	-2.774694000	-0.418303000	-0.288904000
C	-3.590355000	-0.891206000	0.745306000
C	-3.211085000	0.503808000	-1.247814000
C	-4.887725000	-0.390457000	0.810796000
C	-4.517155000	0.969914000	-1.132833000
C	-5.346096000	0.531091000	-0.114313000
H	-5.550203000	-0.733858000	1.596749000
H	-4.892972000	1.682850000	-1.857217000
C	-2.344586000	0.955605000	-2.403239000
H	-1.310497000	0.674589000	-2.189945000
C	-3.136308000	-1.939669000	1.737816000
H	-2.055374000	-2.061145000	1.638409000
C	2.333890000	-0.157836000	-2.372728000
H	1.258987000	0.008827000	-2.262430000
C	1.760306000	-2.295432000	2.227785000
H	0.728433000	-1.972562000	2.079537000
C	-0.300515000	0.793138000	0.991232000
O	-0.222003000	0.347488000	2.265145000
H	-0.759417000	1.334542000	3.337356000
C	0.745747000	1.821259000	0.646974000
C	1.780479000	2.333275000	1.358290000
O	0.585995000	2.526558000	-0.504224000
C	2.299100000	3.422008000	0.591638000
H	2.121279000	1.983307000	2.319214000
C	1.536787000	3.493627000	-0.523849000
H	3.126751000	4.067550000	0.842764000
H	1.540203000	4.139995000	-1.386798000
O	-1.083090000	1.947896000	4.078419000
C	-2.111658000	2.754850000	3.570636000
H	-2.467119000	3.419035000	4.363902000
H	-1.776642000	3.385823000	2.734687000
H	-2.972384000	2.166963000	3.220185000
H	-1.264659000	1.292674000	0.749149000
C	2.132509000	-1.931198000	3.660944000

H	1.415580000	-2.383924000	4.350338000
H	3.124010000	-2.301840000	3.932941000
H	2.113869000	-0.850448000	3.813493000
C	1.837137000	-3.810896000	2.028276000
H	1.182426000	-4.317951000	2.741953000
H	1.534206000	-4.105617000	1.021011000
H	2.857753000	-4.169325000	2.190990000
C	-3.412873000	-1.531747000	3.182566000
H	-4.484640000	-1.453771000	3.380641000
H	-3.006213000	-2.285299000	3.861538000
H	-2.948662000	-0.572742000	3.421118000
C	-3.788692000	-3.287168000	1.424401000
H	-3.425098000	-4.051058000	2.116377000
H	-4.875288000	-3.224080000	1.529769000
H	-3.566604000	-3.614799000	0.406185000
C	-2.369983000	2.469055000	-2.596603000
H	-3.357385000	2.819167000	-2.906715000
H	-2.092443000	2.992927000	-1.679848000
H	-1.660824000	2.751731000	-3.378368000
C	-2.760887000	0.238575000	-3.688794000
H	-2.704612000	-0.846916000	-3.578742000
H	-3.787820000	0.499337000	-3.959426000
H	-2.107109000	0.533511000	-4.513517000
C	2.534712000	-1.280380000	-3.394492000
H	3.601500000	-1.465494000	-3.548396000
H	2.073564000	-2.216590000	-3.075492000
H	2.097700000	-0.995969000	-4.355110000
C	2.944166000	1.134899000	-2.905400000
H	2.878264000	1.943838000	-2.176411000
H	3.994880000	1.001661000	-3.174365000
H	2.413520000	1.443624000	-3.809307000
H	-6.360863000	0.907171000	-0.044704000
H	5.867755000	-0.821777000	0.588745000
H	-1.937169000	-2.744283000	-1.494738000
H	0.795469000	-3.133966000	-1.294111000

IPr-TS2-A $i1107\text{ cm}^{-1}$ Etot = -1617.802519528987 a.u.

C	-0.393455000	-0.295381000	0.082781000
C	-1.203416000	-2.269081000	-0.561610000
H	-1.970557000	-2.988377000	-0.788779000
C	0.137855000	-2.350658000	-0.608408000
H	0.793801000	-3.153739000	-0.895639000
N	-1.526820000	-0.993580000	-0.137749000
N	0.632425000	-1.125772000	-0.212322000
C	2.021807000	-0.776816000	-0.283998000

C	2.868242000	-1.156386000	0.757593000
C	2.485872000	-0.137573000	-1.435541000
C	4.212823000	-0.828191000	0.647875000
C	3.841214000	0.168092000	-1.489393000
C	4.714728000	-0.154161000	-0.459187000
H	4.885187000	-1.109392000	1.452351000
H	4.222714000	0.668802000	-2.373653000
C	-2.902053000	-0.582768000	-0.028285000
C	-3.556570000	-0.746449000	1.188661000
C	-3.547904000	-0.123077000	-1.174342000
C	-4.907291000	-0.431029000	1.243664000
C	-4.900279000	0.180231000	-1.063034000
C	-5.595516000	0.036920000	0.130704000
H	-5.433060000	-0.549297000	2.186197000
H	-5.422065000	0.544256000	-1.942665000
C	-2.816558000	0.088717000	-2.462024000
H	-2.118816000	0.935315000	-2.380687000
H	-2.235362000	-0.791156000	-2.751575000
H	-3.521559000	0.303168000	-3.265850000
C	-2.824630000	-1.192553000	2.415272000
H	-2.200606000	-2.070457000	2.230935000
H	-2.170383000	-0.392008000	2.772971000
H	-3.524603000	-1.435399000	3.214968000
C	2.359389000	-1.905072000	1.949893000
H	1.573576000	-1.343021000	2.458817000
H	1.941211000	-2.876236000	1.670599000
H	3.165548000	-2.080232000	2.662176000
C	1.583489000	0.189856000	-2.583542000
H	1.000604000	-0.683707000	-2.889853000
H	0.864822000	0.987186000	-2.345692000
H	2.173076000	0.514358000	-3.441295000
C	6.161795000	0.227199000	-0.532220000
H	6.792752000	-0.497827000	-0.014805000
H	6.502193000	0.303837000	-1.566112000
H	6.327977000	1.200563000	-0.060204000
C	-7.044826000	0.406680000	0.224733000
H	-7.157763000	1.452267000	0.527528000
H	-7.549368000	0.288816000	-0.735756000
H	-7.565892000	-0.204985000	0.963599000
C	-0.272018000	1.127648000	0.416126000
O	-1.527516000	1.711209000	0.663471000
C	0.726932000	1.446964000	1.463960000
H	-1.630317000	2.252311000	-0.158619000
C	0.798742000	1.187456000	2.797419000
O	1.751705000	2.267960000	1.113235000
C	1.938399000	1.881901000	3.292155000

H	0.100152000	0.592749000	3.365005000
C	2.473836000	2.515733000	2.221082000
H	2.305665000	1.912543000	4.305645000
H	3.332032000	3.154914000	2.095262000
H	-0.034581000	1.691090000	-0.633189000
O	-0.670736000	2.434046000	-1.707815000
C	-0.168260000	3.682561000	-2.010115000
H	0.288410000	4.191585000	-1.140592000
H	0.615281000	3.649730000	-2.791280000
H	-0.950667000	4.364054000	-2.388075000

IPr-III-A Etot = -1617.829199060855 a.u.

C	-0.363370000	-0.340453000	-0.013573000
C	-1.147318000	-2.248245000	-0.952033000
H	-1.892153000	-2.953506000	-1.278611000
C	0.184512000	-2.269879000	-1.064376000
H	0.843907000	-3.014641000	-1.475230000
N	-1.503521000	-1.067773000	-0.310180000
N	0.686691000	-1.105934000	-0.488412000
C	2.085084000	-0.942265000	-0.255906000
C	2.913652000	-0.639186000	-1.346262000
C	2.598631000	-1.167360000	1.027964000
C	4.282639000	-0.546737000	-1.117179000
C	3.973645000	-1.039717000	1.208948000
C	4.810023000	-0.731601000	0.149947000
H	4.946570000	-0.319170000	-1.943832000
H	4.397153000	-1.207808000	2.193054000
C	-2.848486000	-0.586246000	-0.323828000
C	-3.754579000	-1.084956000	0.621994000
C	-3.238827000	0.313144000	-1.324813000
C	-5.073189000	-0.645839000	0.555554000
C	-4.565815000	0.736485000	-1.337143000
C	-5.476233000	0.264266000	-0.407785000
H	-5.795978000	-1.019227000	1.272448000
H	-4.893081000	1.436180000	-2.098647000
C	-2.293638000	0.805307000	-2.399950000
H	-1.311101000	0.365175000	-2.220345000
C	-3.344708000	-2.088300000	1.677493000
H	-2.253305000	-2.140819000	1.677137000
C	2.374156000	-0.432402000	-2.745995000
H	1.283853000	-0.403361000	-2.683981000
C	1.735158000	-1.608512000	2.190012000
H	0.690132000	-1.541811000	1.884109000
C	-0.344435000	0.860514000	0.669167000
O	-1.465492000	1.138349000	1.456383000

H	-1.429694000	1.075192000	3.310639000
C	0.654464000	1.876839000	0.708184000
C	0.783108000	2.966802000	1.538920000
O	1.618580000	1.932290000	-0.248940000
C	1.899557000	3.711079000	1.058068000
H	0.162595000	3.195556000	2.389762000
C	2.376922000	3.042543000	-0.016317000
H	2.300738000	4.625825000	1.468008000
H	3.203697000	3.199571000	-0.689430000
O	-1.509668000	0.942556000	4.271372000
C	-1.069252000	2.106972000	4.935392000
H	-1.237367000	1.965032000	6.004469000
H	0.000580000	2.291547000	4.779680000
H	-1.624042000	2.997753000	4.617570000
H	-1.945049000	1.893444000	1.091453000
H	-6.507026000	0.600408000	-0.438901000
H	5.879432000	-0.646773000	0.310229000
C	2.020141000	-3.069573000	2.540464000
H	1.360682000	-3.400124000	3.347375000
H	1.860347000	-3.723256000	1.679493000
H	3.053348000	-3.196953000	2.875403000
C	1.909570000	-0.713290000	3.413737000
H	1.692145000	0.330019000	3.173964000
H	1.229007000	-1.029475000	4.208303000
H	2.927537000	-0.768956000	3.808217000
C	-3.786331000	-1.672838000	3.078289000
H	-4.875597000	-1.664215000	3.168463000
H	-3.401660000	-2.384218000	3.813809000
H	-3.413298000	-0.680742000	3.339353000
C	-3.881799000	-3.480475000	1.342165000
H	-3.547339000	-3.817268000	0.358472000
H	-3.541961000	-4.206963000	2.085072000
H	-4.975673000	-3.481871000	1.344434000
C	-2.751547000	0.345087000	-3.783754000
H	-2.840433000	-0.742963000	-3.830482000
H	-3.722416000	0.776052000	-4.042523000
H	-2.031265000	0.661734000	-4.542690000
C	-2.131041000	2.323364000	-2.359603000
H	-1.409336000	2.644940000	-3.115032000
H	-3.078545000	2.828008000	-2.566887000
H	-1.773313000	2.659571000	-1.383426000
C	2.762836000	-1.597272000	-3.657884000
H	2.331229000	-1.459372000	-4.652778000
H	3.849504000	-1.655288000	-3.767697000
H	2.413764000	-2.554761000	-3.265152000
C	2.832100000	0.889630000	-3.358177000

H	2.546764000	1.737435000	-2.733793000
H	3.916296000	0.913938000	-3.494563000
H	2.373509000	1.019940000	-4.341916000

IPr-IV-A Etot = -1960.940228049920 a.u.

C	0.671260000	-1.701386000	-0.292241000
C	-0.469518000	0.215479000	-0.276884000
C	0.807183000	0.499923000	0.034375000
H	1.291328000	1.432281000	0.269058000
N	-0.551948000	-1.143794000	-0.472154000
N	1.501496000	-0.684211000	0.025515000
C	2.907759000	-0.664611000	0.380070000
C	3.841156000	-0.347621000	-0.608471000
C	3.248733000	-0.808605000	1.730739000
C	5.173662000	-0.230965000	-0.214361000
C	4.589868000	-0.673863000	2.067217000
C	5.547889000	-0.397114000	1.105114000
H	5.924756000	0.009723000	-0.957678000
H	4.889154000	-0.782836000	3.103063000
C	-1.864245000	-1.718895000	-0.712545000
C	-2.384650000	-1.710944000	-2.010678000
C	-2.627971000	-2.100131000	0.403820000
C	-3.667516000	-2.226895000	-2.188806000
C	-3.903934000	-2.596653000	0.165270000
C	-4.413348000	-2.681990000	-1.119502000
H	-4.093663000	-2.246624000	-3.184865000
H	-4.514418000	-2.912118000	1.002313000
C	-2.150889000	-1.921401000	1.830479000
H	-1.060988000	-1.848208000	1.825979000
C	-1.687444000	-1.079906000	-3.194595000
H	-0.665469000	-0.835577000	-2.902857000
C	3.471310000	-0.069666000	-2.048636000
H	2.429210000	-0.356173000	-2.198842000
C	2.224740000	-1.059996000	2.814782000
H	1.296543000	-1.382706000	2.339706000
H	-1.336272000	0.846935000	-0.370305000
C	1.140105000	-3.163709000	-0.403962000
O	2.262345000	-3.327032000	0.387206000
C	1.488754000	-3.477913000	-1.826670000
C	0.053212000	-4.189968000	0.291207000
H	1.797860000	-3.834280000	1.176220000
C	1.374950000	-2.839500000	-3.018406000
O	2.109415000	-4.669853000	-2.012689000
O	0.523833000	-4.403898000	1.545633000
H	-0.915095000	-3.678337000	0.264492000

C	-0.132049000	-5.464761000	-0.469432000
C	1.944190000	-3.700942000	-4.002925000
H	0.959066000	-1.862967000	-3.190642000
C	2.373399000	-4.794117000	-3.333057000
C	0.193622000	-6.752580000	-0.193077000
O	-0.804641000	-5.404999000	-1.648082000
H	2.028330000	-3.519261000	-5.063011000
H	2.871544000	-5.702342000	-3.632349000
C	-0.295491000	-7.536575000	-1.282980000
H	0.716599000	-7.096985000	0.684306000
C	-0.888803000	-6.668681000	-2.135089000
H	-0.219331000	-8.605660000	-1.410594000
H	-1.400533000	-6.782021000	-3.077366000
H	-0.000173000	-5.550764000	2.595468000
O	-0.275437000	-6.203388000	3.294500000
C	0.140095000	-5.707429000	4.542146000
H	1.231458000	-5.600509000	4.606013000
H	-0.308543000	-4.731751000	4.773071000
H	-0.172677000	-6.411167000	5.317818000
H	-5.409202000	-3.078975000	-1.281982000
H	6.589441000	-0.298119000	1.390368000
C	2.644974000	-2.169528000	3.774335000
H	1.830818000	-2.379799000	4.472193000
H	2.882684000	-3.091403000	3.240321000
H	3.517824000	-1.881964000	4.365340000
C	1.933296000	0.229302000	3.585028000
H	1.588254000	1.027106000	2.923457000
H	1.160727000	0.052465000	4.337809000
H	2.832532000	0.581266000	4.098256000
C	-2.519869000	-3.089703000	2.738621000
H	-3.599570000	-3.158158000	2.889686000
H	-2.161851000	-4.039448000	2.338509000
H	-2.062135000	-2.943966000	3.719922000
C	-2.705724000	-0.615398000	2.405951000
H	-2.327117000	-0.463583000	3.419897000
H	-2.424244000	0.251104000	1.804617000
H	-3.797528000	-0.654359000	2.452667000
C	-1.634208000	-2.004767000	-4.407226000
H	-1.034557000	-1.546192000	-5.197315000
H	-1.190806000	-2.970346000	-4.158671000
H	-2.633066000	-2.181173000	-4.813104000
C	-2.371897000	0.239152000	-3.562284000
H	-3.402995000	0.064359000	-3.880375000
H	-2.390603000	0.933472000	-2.719334000
H	-1.838963000	0.717837000	-4.387671000
C	4.315608000	-0.880990000	-3.027358000

H	4.25545000	-1.949914000	-2.815055000
H	3.959733000	-0.717712000	-4.047576000
H	5.365736000	-0.580928000	-2.991684000
C	3.587208000	1.425149000	-2.352275000
H	3.278707000	1.624471000	-3.381749000
H	2.959809000	2.022157000	-1.686462000
H	4.620333000	1.764243000	-2.237119000

IPr-V-A Etot = -1960.943099427773 a.u.

C	0.615898000	-1.713322000	-0.293292000
C	-0.464981000	0.241167000	-0.296357000
C	0.816964000	0.485084000	0.026256000
H	1.328560000	1.402265000	0.262346000
N	-0.588437000	-1.116311000	-0.487374000
N	1.471506000	-0.722232000	0.032855000
C	2.864592000	-0.741594000	0.434898000
C	3.841595000	-0.464954000	-0.522566000
C	3.150803000	-0.853605000	1.801154000
C	5.159045000	-0.355138000	-0.079579000
C	4.479670000	-0.730468000	2.187177000
C	5.479339000	-0.491019000	1.257652000
H	5.942246000	-0.146281000	-0.799210000
H	4.735881000	-0.817322000	3.236817000
C	-1.914048000	-1.651658000	-0.741469000
C	-2.432067000	-1.599455000	-2.040369000
C	-2.690195000	-2.044928000	0.362969000
C	-3.725301000	-2.082674000	-2.234532000
C	-3.975374000	-2.509069000	0.108089000
C	-4.483267000	-2.550240000	-1.179367000
H	-4.148999000	-2.067747000	-3.231720000
H	-4.594207000	-2.834499000	0.934960000
C	-2.212783000	-1.912036000	1.794363000
H	-1.121136000	-1.920569000	1.797012000
C	-1.720105000	-0.953960000	-3.208183000
H	-0.693441000	-0.737365000	-2.910405000
C	3.532430000	-0.237330000	-1.985480000
H	2.491379000	-0.511489000	-2.163150000
C	2.082301000	-1.065766000	2.850003000
H	1.157869000	-1.346161000	2.342289000
H	-1.309769000	0.900498000	-0.398230000
C	1.081018000	-3.200055000	-0.384503000
O	2.165618000	-3.356635000	0.399101000
C	1.383395000	-3.515496000	-1.830844000
C	-0.063484000	-4.152582000	0.232401000
H	1.195896000	-3.931987000	1.559528000

C	1.264557000	-2.863908000	-3.015119000
O	1.995559000	-4.708845000	-2.037598000
O	0.227070000	-4.196050000	1.595484000
H	-1.045023000	-3.709347000	0.061221000
C	-0.105057000	-5.531799000	-0.328999000
C	1.821649000	-3.716711000	-4.015084000
H	0.853899000	-1.882442000	-3.171418000
C	2.248426000	-4.820259000	-3.360967000
C	0.342623000	-6.728980000	0.126255000
O	-0.745268000	-5.698815000	-1.513907000
H	1.898248000	-3.523936000	-5.073885000
H	2.735492000	-5.729641000	-3.674832000
C	-0.030736000	-7.697214000	-0.855684000
H	0.872698000	-6.897796000	1.049870000
C	-0.683959000	-7.017469000	-1.826485000
H	0.157275000	-8.759820000	-0.835872000
H	-1.154752000	-7.308911000	-2.751580000
H	3.658908000	-3.994160000	0.106464000
O	4.587992000	-4.339380000	0.045919000
C	4.905982000	-4.962248000	1.265017000
H	4.907015000	-4.256449000	2.106809000
H	4.212405000	-5.778155000	1.508725000
H	5.909616000	-5.387709000	1.185272000
H	-5.486525000	-2.922551000	-1.354371000
H	6.510164000	-0.398388000	1.581485000
C	2.425867000	-2.201000000	3.810270000
H	1.586097000	-2.380131000	4.486397000
H	2.635818000	-3.126284000	3.270547000
H	3.296661000	-1.958484000	4.424364000
C	1.819703000	0.227987000	3.622494000
H	1.530602000	1.044377000	2.956588000
H	1.015264000	0.078626000	4.347524000
H	2.714507000	0.538833000	4.168996000
C	-2.668679000	-3.057945000	2.691603000
H	-3.748153000	-3.035009000	2.859197000
H	-2.401424000	-4.028797000	2.272331000
H	-2.185972000	-2.966975000	3.667321000
C	-2.680244000	-0.576218000	2.379194000
H	-2.298902000	-0.460591000	3.396997000
H	-2.335900000	0.275235000	1.789502000
H	-3.772523000	-0.540333000	2.419014000
C	-1.685705000	-1.848510000	-4.444382000
H	-1.074821000	-1.382966000	-5.221705000
H	-1.264938000	-2.830295000	-4.221491000
H	-2.687598000	-1.991505000	-4.855801000
C	-2.377961000	0.386842000	-3.545042000

H	-3.411278000	0.239115000	-3.869576000
H	-2.386295000	1.061487000	-2.686210000
H	-1.833966000	0.874729000	-4.357715000
C	4.394183000	-1.108159000	-2.895864000
H	4.302756000	-2.165394000	-2.639497000
H	4.080783000	-0.982947000	-3.935236000
H	5.449027000	-0.829656000	-2.832280000
C	3.691235000	1.240120000	-2.347150000
H	3.429050000	1.401865000	-3.395941000
H	3.049332000	1.875933000	-1.732879000
H	4.725470000	1.564809000	-2.203384000

VI...IPr-I(H)-A Etot = -1960.954576544535 a.u.

C	-1.883557000	0.584439000	-0.314379000
C	-2.711256000	1.748563000	-2.080304000
H	-3.470497000	2.233295000	-2.671542000
C	-1.385218000	1.600464000	-2.283007000
N	-2.988181000	1.124640000	-0.880731000
N	-0.905782000	0.892918000	-1.198544000
C	0.469244000	0.530449000	-1.037465000
C	1.343769000	1.455152000	-0.453931000
C	0.892763000	-0.724284000	-1.490688000
C	2.679730000	1.085693000	-0.323499000
C	2.238469000	-1.046170000	-1.334301000
C	3.124083000	-0.152369000	-0.756368000
H	3.383078000	1.780447000	0.121885000
H	2.597776000	-2.010376000	-1.676693000
C	-4.296928000	1.053476000	-0.305590000
C	-5.131093000	-0.011926000	-0.663557000
C	-4.697071000	2.056837000	0.584271000
C	-6.402440000	-0.054554000	-0.097654000
C	-5.977503000	1.967225000	1.123863000
C	-6.823146000	0.923612000	0.787567000
H	-7.072299000	-0.867722000	-0.354837000
H	-6.316499000	2.728427000	1.817928000
C	-3.799672000	3.213601000	0.966637000
H	-2.847154000	3.090425000	0.447049000
C	-4.701601000	-1.092297000	-1.631947000
H	-3.666088000	-0.898259000	-1.919021000
C	0.891300000	2.826983000	-0.002240000
H	-0.198612000	2.861082000	-0.064438000
C	-0.043224000	-1.706159000	-2.161168000
H	-1.056508000	-1.304143000	-2.099296000
H	-0.748926000	1.929966000	-3.087603000
H	-1.978213000	-0.357154000	1.191807000

O	-2.149990000	-0.916766000	2.025057000
C	-0.936619000	-1.358920000	2.546598000
C	-0.278670000	-0.316475000	3.460604000
H	-0.222363000	-1.578277000	1.740106000
C	-1.130721000	-2.617216000	3.323042000
O	-0.936010000	0.578209000	3.965875000
C	1.146442000	-0.445659000	3.690902000
C	-1.413468000	-2.880676000	4.624202000
O	-1.074288000	-3.777937000	2.620500000
C	2.106589000	-1.285311000	3.194259000
O	1.715938000	0.426549000	4.566660000
C	-1.543584000	-4.297611000	4.730269000
H	-1.517779000	-2.152864000	5.414427000
C	-1.329037000	-4.786459000	3.486039000
C	3.326233000	-0.905709000	3.800290000
H	1.956555000	-2.078534000	2.478296000
C	3.022926000	0.136797000	4.621086000
H	-1.765205000	-4.872880000	5.615695000
H	-1.319312000	-5.781526000	3.070992000
H	4.300840000	-1.342277000	3.650022000
H	3.618691000	0.748130000	5.280841000
O	-0.327587000	3.063429000	5.169647000
C	-0.077621000	2.941936000	6.553242000
H	-0.443008000	2.171687000	4.801044000
H	-0.906472000	2.454398000	7.080480000
H	0.840936000	2.378966000	6.757674000
H	0.040803000	3.947272000	6.961417000
H	-7.817218000	0.872296000	1.218323000
H	4.168952000	-0.421239000	-0.645125000
C	-4.743375000	-2.475001000	-0.984441000
H	-5.762399000	-2.749796000	-0.699626000
H	-4.378450000	-3.228920000	-1.686770000
H	-4.118833000	-2.512003000	-0.088795000
C	-5.546492000	-1.059027000	-2.904693000
H	-5.490294000	-0.083129000	-3.392964000
H	-5.193957000	-1.815155000	-3.610993000
H	-6.597026000	-1.268103000	-2.685391000
C	0.303527000	-1.860044000	-3.641921000
H	-0.405164000	-2.535995000	-4.127523000
H	0.268651000	-0.898710000	-4.160162000
H	1.306773000	-2.276639000	-3.767506000
C	-0.048108000	-3.062403000	-1.460257000
H	-0.316765000	-2.964284000	-0.405987000
H	-0.774732000	-3.725817000	-1.936400000
H	0.930485000	-3.546052000	-1.517725000
C	-4.397263000	4.547812000	0.522905000

H	-4.580877000	4.562319000	-0.554199000
H	-5.345360000	4.744351000	1.030852000
H	-3.712675000	5.365220000	0.763768000
C	-3.505068000	3.217634000	2.465564000
H	-2.815566000	4.029537000	2.711288000
H	-4.418465000	3.367290000	3.047565000
H	-3.050595000	2.276420000	2.782991000
C	1.443159000	3.908761000	-0.930974000
H	2.536096000	3.928906000	-0.897695000
H	1.139316000	3.738178000	-1.966569000
H	1.077827000	4.892530000	-0.624998000
C	1.272657000	3.112848000	1.447834000
H	0.866769000	2.356777000	2.123016000
H	2.357232000	3.139888000	1.580307000
H	0.877775000	4.085709000	1.751446000

IPr-I(H)-B Etot = -1274.183967992810 a.u.

C	-0.241441000	-0.669413000	0.250475000
C	-0.714871000	1.453302000	-0.418519000
H	-1.386201000	2.264911000	-0.660242000
C	0.649180000	1.395170000	-0.441773000
H	1.891459000	2.444279000	-0.916526000
N	-1.226763000	0.220793000	-0.006165000
N	0.870347000	0.068974000	-0.021413000
C	2.178137000	-0.479384000	0.112837000
C	2.771367000	-1.114149000	-0.986804000
C	2.847002000	-0.364847000	1.339012000
C	4.049403000	-1.645652000	-0.831823000
C	4.123415000	-0.911309000	1.448477000
C	4.722576000	-1.549106000	0.374853000
H	4.524029000	-2.144586000	-1.670420000
H	4.656127000	-0.835485000	2.390769000
C	-2.614708000	-0.067332000	0.119326000
C	-3.312136000	-0.558643000	-0.992768000
C	-3.253451000	0.166959000	1.344599000
C	-4.671303000	-0.825867000	-0.849700000
C	-4.613813000	-0.115187000	1.440241000
C	-5.319355000	-0.608085000	0.354911000
H	-5.230211000	-1.212192000	-1.695582000
H	-5.128290000	0.053302000	2.380459000
C	-2.508138000	0.700246000	2.548472000
H	-1.475720000	0.881626000	2.243032000
C	-2.631761000	-0.810973000	-2.320452000
H	-1.587241000	-0.509458000	-2.219182000
C	2.064760000	-1.237445000	-2.319309000

H	1.100161000	-0.734917000	-2.226236000
C	2.224840000	0.330541000	2.530178000
H	1.239738000	0.687278000	2.224031000
O	2.665992000	3.082203000	-1.217867000
C	2.086150000	4.255034000	-1.713366000
H	2.874033000	4.953400000	-2.013821000
H	1.453564000	4.074985000	-2.596353000
H	1.462441000	4.767450000	-0.964589000
H	5.717203000	-1.969821000	0.478107000
H	-6.378586000	-0.822841000	0.448101000
C	2.027027000	-0.631421000	3.699968000
H	2.984253000	-1.016920000	4.062105000
H	1.535679000	-0.120625000	4.532708000
H	1.407509000	-1.483727000	3.410157000
C	3.045109000	1.546575000	2.956944000
H	3.160762000	2.253655000	2.131655000
H	2.551915000	2.065069000	3.783778000
H	4.043429000	1.253720000	3.294236000
C	2.843638000	-0.541612000	-3.433990000
H	2.288211000	-0.595662000	-4.374350000
H	3.013579000	0.511770000	-3.198298000
H	3.817043000	-1.013690000	-3.594097000
C	1.794811000	-2.698478000	-2.674018000
H	2.728534000	-3.255036000	-2.795410000
H	1.205872000	-3.191619000	-1.896722000
H	1.241405000	-2.764957000	-3.614867000
C	-2.480503000	-0.324047000	3.681743000
H	-1.897168000	0.058140000	4.523942000
H	-3.489722000	-0.539971000	4.043783000
H	-2.030073000	-1.264049000	3.353844000
C	-3.089845000	2.028183000	3.028950000
H	-3.083682000	2.775342000	2.231489000
H	-4.120868000	1.909955000	3.373755000
H	-2.501807000	2.417152000	3.864544000
C	-2.650972000	-2.295756000	-2.679772000
H	-2.174283000	-2.897019000	-1.901732000
H	-3.675066000	-2.657549000	-2.807711000
H	-2.115715000	-2.465770000	-3.617929000
C	-3.250568000	0.027085000	-3.437423000
H	-2.709612000	-0.133441000	-4.373880000
H	-4.296281000	-0.244831000	-3.605733000
H	-3.212513000	1.093222000	-3.200666000

IPr-I(H2)-B Etot = -1389.843324681597a.u.

C	-0.234288000000	-0.683977000000	0.211102000000
C	-0.704404000000	1.430067000000	-0.453224000000
H	-1.374299000000	2.242866000000	-0.693805000000
C	0.660336000000	1.368989000000	-0.478326000000
H	1.897565000000	2.469069000000	-0.907810000000
N	-1.220562000000	0.200747000000	-0.042384000000
N	0.880483000000	0.043269000000	-0.060319000000
C	2.187172000000	-0.513358000000	0.065652000000
C	2.783582000000	-1.115331000000	-1.050763000000
C	2.849894000000	-0.434318000000	1.297736000000
C	4.062120000000	-1.648367000000	-0.906641000000
C	4.127109000000	-0.981404000000	1.394808000000
C	4.730846000000	-1.585530000000	0.304656000000
H	4.541338000000	-2.120735000000	-1.757823000000
H	4.657460000000	-0.931133000000	2.339997000000
C	-2.609997000000	-0.088947000000	0.079929000000
C	-3.306167000000	-0.560611000000	-1.041185000000
C	-3.247560000000	0.126602000000	1.308832000000
C	-4.666556000000	-0.824291000000	-0.904115000000
C	-4.609305000000	-0.150973000000	1.397250000000
C	-5.315114000000	-0.622815000000	0.302987000000
H	-5.226214000000	-1.194049000000	-1.756801000000
H	-5.124486000000	0.005535000000	2.339017000000
C	-2.505871000000	0.646779000000	2.520517000000
H	-1.457006000000	0.765454000000	2.241175000000
C	-2.626772000000	-0.788110000000	-2.374015000000
H	-1.574549000000	-0.519275000000	-2.260912000000
C	2.086056000000	-1.194687000000	-2.391613000000
H	1.104174000000	-0.730740000000	-2.280288000000
C	2.227393000000	0.232277000000	2.505259000000
H	1.225719000000	0.560386000000	2.221320000000
O	2.647961000000	3.142323000000	-1.171437000000
C	2.032191000000	4.299066000000	-1.663088000000
H	2.799030000000	5.029074000000	-1.940941000000
H	1.422898000000	4.105915000000	-2.559206000000
H	1.377324000000	4.777825000000	-0.919087000000
H	5.726242000000	-2.006542000000	0.398480000000
H	-6.375432000000	-0.834070000000	0.391258000000
C	2.082374000000	-0.739763000000	3.674338000000
H	3.057913000000	-1.088988000000	4.023932000000
H	1.583385000000	-0.248861000000	4.514363000000
H	1.491788000000	-1.614378000000	3.391034000000
C	3.019655000000	1.470529000000	2.922268000000
H	3.096186000000	2.186278000000	2.100001000000
H	2.530200000000	1.968481000000	3.763752000000
H	4.033349000000	1.203684000000	3.234360000000

C	2.848105000000	-0.414191000000	-3.461566000000
H	2.301632000000	-0.438002000000	-4.408357000000
H	2.981044000000	0.630264000000	-3.170029000000
H	3.837847000000	-0.845629000000	-3.635938000000
C	1.869958000000	-2.641825000000	-2.829718000000
H	2.822989000000	-3.156111000000	-2.982383000000
H	1.299387000000	-3.202321000000	-2.085381000000
H	1.319795000000	-2.672436000000	-3.774258000000
C	-2.564226000000	-0.343944000000	3.681690000000
H	-1.970994000000	0.025340000000	4.522597000000
H	-3.590236000000	-0.483711000000	4.033151000000
H	-2.170591000000	-1.320279000000	3.389341000000
C	-3.030891000000	2.016698000000	2.946967000000
H	-2.958273000000	2.740440000000	2.131478000000
H	-4.078254000000	1.959195000000	3.256399000000
H	-2.452134000000	2.397018000000	3.792956000000
C	-2.685983000000	-2.257337000000	-2.787742000000
H	-2.225900000000	-2.901169000000	-2.034067000000
H	-3.718792000000	-2.587333000000	-2.929912000000
H	-2.154771000000	-2.405491000000	-3.731861000000
C	-3.219194000000	0.107081000000	-3.460943000000
H	-2.681594000000	-0.035307000000	-4.402197000000
H	-4.272076000000	-0.129108000000	-3.638255000000
H	-3.151229000000	1.162449000000	-3.185840000000
H	-0.440972000000	-2.292764000000	0.986841000000
O	-0.588509000000	-3.172767000000	1.470705000000
C	-0.228414000000	-4.218151000000	0.607093000000
H	0.853976000000	-4.252497000000	0.416695000000
H	-0.514628000000	-5.170310000000	1.062698000000
H	-0.734932000000	-4.148814000000	-0.365715000000

IPr-I-B Etot = -1158.516467465710 a.u.

C	-0.330215000	-0.709885000	0.253419000
C	-0.588938000	1.470764000	-0.402664000
H	-1.189278000	2.334614000	-0.651212000
C	0.767004000	1.310488000	-0.385881000
N	-1.224281000	0.267283000	-0.021967000
N	0.844514000	-0.045907000	0.024525000
C	2.094478000	-0.696590000	0.195414000
C	2.656475000	-1.404898000	-0.875166000
C	2.756037000	-0.605611000	1.426855000
C	3.893192000	-2.015830000	-0.693149000
C	3.991719000	-1.230158000	1.566764000
C	4.560314000	-1.930470000	0.517010000
H	4.342566000	-2.569675000	-1.510254000

H	4.517593000	-1.170409000	2.513620000
C	-2.626120000	0.100189000	0.059380000
C	-3.336447000	-0.311343000	-1.077028000
C	-3.284057000	0.384048000	1.264282000
C	-4.717935000	-0.446271000	-0.982282000
C	-4.666456000	0.235382000	1.315429000
C	-5.381073000	-0.176344000	0.203037000
H	-5.285650000	-0.768016000	-1.848628000
H	-5.194072000	0.445253000	2.239509000
C	-2.491703000	0.786381000	2.487747000
H	-1.556175000	1.222574000	2.127118000
C	-2.599569000	-0.654887000	-2.352012000
H	-1.653608000	-0.107186000	-2.326586000
C	1.948876000	-1.455997000	-2.210315000
H	0.882281000	-1.348987000	-1.998100000
C	2.155914000	0.194011000	2.560887000
H	1.078074000	0.221437000	2.383773000
H	5.523635000	-2.414726000	0.643266000
H	-6.459490000	-0.285025000	0.259458000
C	2.383808000	-0.432622000	3.931309000
H	3.438448000	-0.412742000	4.223422000
H	1.829615000	0.124876000	4.692200000
H	2.044619000	-1.471191000	3.956828000
C	2.664985000	1.634919000	2.516717000
H	2.420027000	2.084080000	1.550498000
H	2.200136000	2.231628000	3.308989000
H	3.750836000	1.665251000	2.660491000
C	2.369677000	-0.266156000	-3.073691000
H	1.822079000	-0.266503000	-4.022369000
H	2.160289000	0.669605000	-2.548352000
H	3.440820000	-0.314352000	-3.299368000
C	2.141465000	-2.772569000	-2.952593000
H	3.174500000	-2.909604000	-3.287597000
H	1.871228000	-3.627448000	-2.327666000
H	1.509856000	-2.791594000	-3.845590000
C	-2.133433000	-0.451504000	3.310685000
H	-1.518279000	-0.175679000	4.173290000
H	-3.038517000	-0.944405000	3.681837000
H	-1.572991000	-1.160623000	2.697167000
C	-3.192047000	1.833043000	3.346149000
H	-3.477434000	2.708432000	2.757411000
H	-4.094074000	1.437620000	3.823302000
H	-2.524152000	2.165578000	4.145581000
C	-2.265951000	-2.146880000	-2.377875000
H	-1.675514000	-2.415307000	-1.498814000
H	-3.181744000	-2.747840000	-2.383678000

H	-1.689488000	-2.397203000	-3.274278000
C	-3.344341000	-0.236859000	-3.614279000
H	-2.713438000	-0.406114000	-4.491237000
H	-4.262283000	-0.814385000	-3.761046000
H	-3.611915000	0.822437000	-3.589196000

IPr-TS1-B $i109\text{ cm}^{-1}$ Etot = -1617.176877669016 a.u.

C	-1.748522000	-1.922574000	-0.166544000
C	-2.256709000	-0.083912000	-1.433986000
H	-2.939694000	0.639309000	-1.856933000
C	-0.899663000	-0.167467000	-1.516519000
H	2.531613000	3.090452000	-0.746615000
N	-2.745046000	-1.130673000	-0.626508000
N	-0.659700000	-1.313147000	-0.721985000
C	0.650340000	-1.819927000	-0.526551000
C	1.555896000	-1.105988000	0.263340000
C	1.030517000	-3.016762000	-1.136233000
C	2.844153000	-1.604138000	0.420511000
C	2.326885000	-3.484816000	-0.944602000
C	3.251392000	-2.790997000	-0.175886000
H	3.548009000	-1.042826000	1.029565000
H	2.621480000	-4.417550000	-1.419723000
C	-4.108296000	-1.335615000	-0.314637000
C	-4.955207000	-1.914056000	-1.262307000
C	-4.601876000	-0.928495000	0.928231000
C	-6.301583000	-2.072470000	-0.949487000
C	-5.952497000	-1.108996000	1.201858000
C	-6.819941000	-1.678542000	0.276996000
H	-6.960851000	-2.524412000	-1.686413000
H	-6.337484000	-0.790303000	2.167378000
C	-3.681643000	-0.319572000	1.938579000
H	-2.916025000	-1.041047000	2.234766000
H	-3.148344000	0.536077000	1.516418000
H	-4.233638000	0.006614000	2.822398000
C	-4.409796000	-2.381849000	-2.575845000
H	-3.978021000	-1.556145000	-3.146440000
H	-3.599946000	-3.098856000	-2.416849000
H	-5.190357000	-2.855013000	-3.174960000
C	1.137907000	0.158653000	0.944185000
H	0.760235000	0.881537000	0.217743000
H	0.317837000	-0.037008000	1.641852000
H	1.973278000	0.599921000	1.490339000
C	0.063801000	-3.777923000	-1.988990000
H	-0.782614000	-4.126220000	-1.392124000
H	-0.351257000	-3.132962000	-2.768560000

H	0.553133000	-4.633274000	-2.460616000
C	4.658416000	-3.289377000	-0.018346000
H	5.040397000	-3.094634000	0.987103000
H	4.721691000	-4.364519000	-0.202220000
H	5.337107000	-2.795438000	-0.722214000
C	-8.268201000	-1.890354000	0.608962000
H	-8.413679000	-2.811218000	1.184044000
H	-8.664163000	-1.068172000	1.210358000
H	-8.875351000	-1.971084000	-0.295428000
O	3.260915000	3.272378000	-0.126082000
C	2.717609000	3.942167000	0.974966000
H	3.534296000	4.180373000	1.662815000
H	2.226194000	4.884605000	0.694036000
H	1.984510000	3.331825000	1.520714000
C	0.549788000	2.235015000	-2.536654000
H	0.915317000	1.205714000	-2.605467000
O	1.037943000	3.075337000	-1.797418000
C	-0.552413000	2.540145000	-3.438641000
C	-1.268290000	1.752703000	-4.291804000
O	-0.962615000	3.831825000	-3.551344000
C	-2.169731000	2.611848000	-4.968702000
H	-1.180933000	0.679591000	-4.348148000
C	-1.936003000	3.856521000	-4.473800000
H	-2.906487000	2.345491000	-5.710061000
H	-2.372365000	4.821374000	-4.676650000

IPr-II-B Etot = -1617.339058061638 a.u.

C	-0.708414000	-0.668209000	0.685626000
C	0.473625000	-1.070036000	0.165520000
N	-1.689332000	-1.019348000	-0.223236000
C	-1.187674000	-1.643368000	-1.316664000
N	0.148052000	-1.657927000	-1.054864000
H	-0.931033000	-0.171409000	1.615936000
O	1.347809000	2.397728000	-0.048583000
C	1.887998000	-0.897574000	0.682736000
O	2.531999000	0.175555000	0.143491000
H	1.795725000	1.470368000	0.049794000
C	2.352106000	3.364848000	-0.165202000
H	3.027641000	3.377859000	0.703534000
H	2.973983000	3.223083000	-1.062150000
H	1.894368000	4.356762000	-0.238623000
H	2.405445000	-1.851030000	0.437236000
C	1.852003000	-0.848357000	2.190734000
C	2.163262000	0.126886000	3.081008000
O	1.468445000	-1.969221000	2.860062000

C	1.951308000	-0.425806000	4.383737000
H	2.505305000	1.118747000	2.832872000
C	1.531503000	-1.696732000	4.188471000
H	2.096586000	0.059741000	5.336812000
H	1.255918000	-2.500118000	4.852916000
C	-3.078074000	-0.758452000	-0.019588000
C	-3.612772000	0.452807000	-0.475447000
C	-3.856300000	-1.714144000	0.644980000
C	-4.966771000	0.690146000	-0.253436000
C	-5.205465000	-1.431136000	0.841809000
C	-5.757758000	-0.241091000	0.398427000
H	-5.407223000	1.620164000	-0.596353000
H	-5.832136000	-2.154828000	1.351873000
C	1.085052000	-2.270955000	-1.944850000
C	1.542450000	-1.552604000	-3.057818000
C	1.489387000	-3.589250000	-1.694900000
C	2.421361000	-2.192213000	-3.928293000
C	2.374463000	-4.182274000	-2.591645000
C	2.837104000	-3.492913000	-3.699451000
H	2.783817000	-1.662234000	-4.802056000
H	2.697278000	-5.203978000	-2.424683000
C	1.087229000	-0.140621000	-3.357166000
H	0.569003000	0.236557000	-2.473151000
C	0.957739000	-4.392012000	-0.526542000
H	0.409155000	-3.712412000	0.128884000
C	-2.772887000	1.492939000	-1.183870000
H	-1.762741000	1.092928000	-1.290032000
C	-3.281086000	-3.020394000	1.147502000
H	-2.222768000	-3.045747000	0.880436000
H	3.522679000	-3.972671000	-4.389734000
H	-6.810618000	-0.038068000	0.562278000
C	2.255848000	0.799539000	-3.642807000
H	2.978546000	0.795402000	-2.824120000
H	2.779564000	0.524300000	-4.561892000
H	1.887907000	1.821358000	-3.767310000
C	0.095030000	-0.128833000	-4.520107000
H	0.568349000	-0.493650000	-5.436440000
H	-0.770352000	-0.760285000	-4.308464000
H	-0.259671000	0.888713000	-4.706098000
C	-3.301699000	1.778430000	-2.587925000
H	-3.342965000	0.866422000	-3.188302000
H	-4.306578000	2.208010000	-2.554536000
H	-2.649715000	2.493036000	-3.097119000
C	-2.676753000	2.778753000	-0.364158000
H	-3.660086000	3.239828000	-0.236210000
H	-2.260838000	2.586394000	0.627776000

H	-2.029928000	3.500787000	-0.869426000
C	-3.951467000	-4.218884000	0.478621000
H	-3.858551000	-4.168135000	-0.608895000
H	-3.486673000	-5.148471000	0.817688000
H	-5.015379000	-4.267144000	0.726220000
C	-3.376239000	-3.120462000	2.669024000
H	-4.418120000	-3.120309000	3.000992000
H	-2.914372000	-4.048791000	3.015404000
H	-2.866349000	-2.284453000	3.153994000
C	-0.026452000	-5.456240000	-1.012803000
H	-0.444967000	-6.003386000	-0.163675000
H	-0.851405000	-5.007278000	-1.571022000
H	0.472966000	-6.177188000	-1.666379000
C	2.073123000	-5.025927000	0.300883000
H	2.782216000	-4.274306000	0.655829000
H	1.649250000	-5.531541000	1.172357000
H	2.628084000	-5.770838000	-0.275141000

IPr -TS2-B $i1101\text{ cm}^{-1}$ Etot = -1617.290398446087 a.u.

C	-0.408939000	-0.837790000	0.436892000
C	0.734513000	-1.224302000	-0.177105000
N	-1.453733000	-1.149182000	-0.406911000
C	-1.031241000	-1.691322000	-1.571257000
N	0.326056000	-1.729705000	-1.412649000
H	-0.569147000	-0.421329000	1.415466000
O	3.803824000	-3.373383000	0.913838000
C	2.111557000	-1.277457000	0.435725000
O	3.172319000	-1.166534000	-0.488270000
H	3.721977000	-1.958212000	-0.200654000
C	4.236392000	-3.559567000	2.191431000
H	5.286535000	-3.233998000	2.382237000
H	3.619966000	-3.018333000	2.957171000
H	4.223506000	-4.624167000	2.505446000
H	2.282162000	-2.262317000	0.931636000
C	2.299170000	-0.248854000	1.522106000
C	3.268029000	0.680363000	1.706622000
O	1.481099000	-0.277237000	2.603500000
C	3.025651000	1.272219000	2.985972000
H	4.062952000	0.908465000	1.017311000
C	1.934376000	0.653067000	3.483846000
H	3.597768000	2.049924000	3.467950000
H	1.379120000	0.750412000	4.401454000
C	-2.817528000	-0.990266000	-0.012735000
C	-3.568564000	0.086727000	-0.494655000
C	-3.343092000	-1.917976000	0.897985000

C	-4.876940000	0.222128000	-0.033772000
C	-4.650598000	-1.732682000	1.337894000
C	-5.413283000	-0.671509000	0.876860000
H	-5.480750000	1.049113000	-0.392557000
H	-5.078744000	-2.433145000	2.046718000
C	1.129102000	-2.034364000	-2.566037000
C	1.350062000	-1.003817000	-3.492973000
C	1.574751000	-3.335183000	-2.797951000
C	2.031290000	-1.307181000	-4.666807000
C	2.241505000	-3.592004000	-3.995791000
C	2.470475000	-2.594528000	-4.924957000
H	2.212056000	-0.522035000	-5.393552000
H	2.595134000	-4.597916000	-4.193425000
C	0.858898000	0.414090000	-3.281861000
H	0.350134000	0.456753000	-2.317787000
C	1.404300000	-4.468757000	-1.814210000
H	0.913442000	-4.071908000	-0.922160000
C	-3.019660000	1.094413000	-1.478175000
H	-2.008600000	0.784847000	-1.738719000
C	-2.538266000	-3.099326000	1.391598000
H	-1.567593000	-3.079800000	0.894039000
H	2.994758000	-2.818918000	-5.847286000
H	-6.431461000	-0.541614000	1.228498000
C	0.499750000	-5.571443000	-2.360525000
H	0.886985000	-5.974267000	-3.298880000
H	0.446126000	-6.392478000	-1.639728000
H	-0.515858000	-5.209640000	-2.535578000
C	2.787108000	-4.992744000	-1.400684000
H	3.209267000	-4.388925000	-0.566656000
H	2.715233000	-6.019516000	-1.020209000
H	3.481570000	-5.004800000	-2.242888000
C	-3.207844000	-4.420585000	1.021087000
H	-3.449025000	-4.455593000	-0.041453000
H	-2.542313000	-5.255853000	1.244862000
H	-4.129502000	-4.569614000	1.587464000
C	-2.269563000	-3.017489000	2.897898000
H	-3.129726000	-3.370992000	3.471957000
H	-1.402910000	-3.628963000	3.161843000
H	-2.057944000	-1.992541000	3.211193000
C	-3.849354000	1.125771000	-2.769838000
H	-3.215137000	1.381160000	-3.621554000
H	-4.315877000	0.159746000	-2.976887000
H	-4.645374000	1.873580000	-2.709110000
C	-2.924923000	2.489281000	-0.859086000
H	-3.841018000	2.749588000	-0.323144000
H	-2.092312000	2.556337000	-0.156253000

H	-2.770722000	3.238138000	-1.640097000
C	2.020204000	1.425597000	-3.240909000
H	2.288227000	1.681711000	-2.211064000
H	2.915366000	1.030429000	-3.728202000
H	1.748201000	2.354906000	-3.754088000
C	-0.160349000	0.797332000	-4.356895000
H	0.328689000	0.961311000	-5.320348000
H	-0.915025000	0.019579000	-4.486643000
H	-0.670524000	1.723896000	-4.080995000

IPr-III-B Etot = -1617.303689204556 a.u.

C	-0.363090000	-0.793136000	0.498634000
C	0.810416000	-1.030322000	-0.188128000
N	-1.408550000	-1.125170000	-0.356677000
C	-0.995391000	-1.546896000	-1.560851000
N	0.370923000	-1.487088000	-1.445915000
H	-0.531394000	-0.458594000	1.505112000
O	2.084600000	-3.479659000	1.842537000
C	2.170078000	-0.936074000	0.240259000
O	3.197918000	-1.099218000	-0.705827000
H	3.497948000	-2.012399000	-0.690156000
C	1.930113000	-3.188999000	3.213811000
H	2.055210000	-4.119672000	3.771638000
H	2.679740000	-2.472852000	3.570839000
H	0.935507000	-2.785259000	3.441243000
H	2.082168000	-2.631438000	1.340165000
C	2.583102000	-0.213734000	1.384648000
C	3.837979000	0.184535000	1.825549000
O	1.650075000	0.184588000	2.303994000
C	3.637444000	0.840471000	3.074007000
H	4.771487000	0.016766000	1.313890000
C	2.309481000	0.818728000	3.332356000
H	4.394835000	1.281354000	3.706457000
H	1.691070000	1.186345000	4.134216000
C	-2.775692000	-1.032523000	0.032306000
C	-3.483142000	0.146084000	-0.235365000
C	-3.367027000	-2.119603000	0.688580000
C	-4.818710000	0.208912000	0.155358000
C	-4.704068000	-2.009257000	1.061933000
C	-5.426282000	-0.857320000	0.797079000
H	-5.390650000	1.108553000	-0.045828000
H	-5.186888000	-2.839769000	1.565983000
C	1.177669000	-1.787378000	-2.588087000
C	1.567637000	-3.111001000	-2.825859000
C	1.498978000	-0.755609000	-3.479198000

C	2.296919000	-3.383622000	-3.980923000
C	2.232397000	-1.074405000	-4.618362000
C	2.630710000	-2.376739000	-4.870975000
H	2.604312000	-4.402897000	-4.188753000
H	2.492799000	-0.289768000	-5.321068000
C	1.197656000	-4.240145000	-1.888896000
H	0.779465000	-3.795162000	-0.983542000
C	1.072811000	0.676875000	-3.242770000
H	0.534982000	0.711880000	-2.293324000
C	-2.845160000	1.329990000	-0.927872000
H	-1.801949000	1.074905000	-1.124836000
C	-2.603977000	-3.391713000	0.986619000
H	-1.581720000	-3.257131000	0.627518000
H	3.199394000	-2.608094000	-5.765388000
H	-6.467592000	-0.789888000	1.093600000
C	0.119303000	-5.127859000	-2.510276000
H	-0.769186000	-4.547388000	-2.768952000
H	0.489254000	-5.607457000	-3.421281000
H	-0.176737000	-5.915007000	-1.811214000
C	2.407207000	-5.076332000	-1.478104000
H	2.847677000	-5.594549000	-2.333823000
H	3.184069000	-4.460223000	-1.018901000
H	2.106436000	-5.835528000	-0.751402000
C	0.116048000	1.156152000	-4.333203000
H	-0.764243000	0.512143000	-4.398850000
H	-0.221204000	2.174704000	-4.122153000
H	0.605221000	1.161410000	-5.311353000
C	2.274823000	1.612686000	-3.128007000
H	1.941001000	2.628664000	-2.900167000
H	2.953685000	1.289204000	-2.336044000
H	2.838999000	1.650005000	-4.064138000
C	-2.534249000	-3.663988000	2.488018000
H	-1.936232000	-4.558445000	2.681991000
H	-2.077219000	-2.826838000	3.021406000
H	-3.530048000	-3.830207000	2.908260000
C	-3.202141000	-4.585023000	0.243775000
H	-3.221206000	-4.410109000	-0.834645000
H	-2.609473000	-5.484106000	0.433071000
H	-4.225836000	-4.783542000	0.573253000
C	-2.859670000	2.572334000	-0.039086000
H	-3.881942000	2.894213000	0.178003000
H	-2.354426000	2.384875000	0.911535000
H	-2.348464000	3.399301000	-0.539182000
C	-3.513054000	1.614959000	-2.271826000
H	-3.473853000	0.740687000	-2.926061000
H	-4.562373000	1.893662000	-2.140638000

H -3.007804000 2.442188000 -2.777582000

IPr-IV-B Etot = -1960.458937824896 a.u.

C	0.524638000	-1.462995000	-0.061865000
C	-0.554350000	0.564064000	0.010702000
C	0.773202000	0.782553000	0.168255000
H	1.323099000	1.700352000	0.295098000
N	-0.674722000	-0.821577000	-0.128232000
N	1.398844000	-0.445093000	0.114939000
C	2.815723000	-0.616981000	0.190264000
C	3.565127000	-0.530436000	-0.990165000
C	3.410827000	-0.859456000	1.434122000
C	4.944128000	-0.699650000	-0.899445000
C	4.793035000	-1.026172000	1.471600000
C	5.554818000	-0.947077000	0.318283000
H	5.548046000	-0.638012000	-1.798272000
H	5.279156000	-1.221753000	2.421230000
C	-1.871555000	-1.598500000	-0.292362000
C	-2.509328000	-2.106510000	0.846717000
C	-2.315996000	-1.897716000	-1.584209000
C	-3.622683000	-2.920129000	0.662744000
C	-3.437449000	-2.714381000	-1.716631000
C	-4.088468000	-3.221719000	-0.606572000
H	-4.131375000	-3.329238000	1.528627000
H	-3.799019000	-2.962983000	-2.708434000
C	-1.609884000	-1.403102000	-2.827522000
H	-0.846746000	-0.686015000	-2.519889000
C	-2.011607000	-1.828299000	2.248376000
H	-1.264977000	-1.033698000	2.188660000
C	2.931788000	-0.262489000	-2.338066000
H	1.851327000	-0.195748000	-2.196358000
C	2.611690000	-0.954145000	2.715076000
H	1.566503000	-0.747353000	2.476302000
C	-1.662290000	1.593722000	-0.092231000
O	-2.915068000	1.047081000	0.197077000
H	-2.946145000	1.258569000	1.179863000
C	-1.656794000	2.182427000	-1.468678000
C	-0.698845000	2.313895000	-2.424952000
O	-2.794195000	2.795896000	-1.880293000
C	-1.284675000	3.063783000	-3.488055000
H	0.304353000	1.922743000	-2.378725000
C	-2.555435000	3.325671000	-3.103474000
H	-0.822039000	3.358258000	-4.417555000
H	-3.382936000	3.838294000	-3.567339000
C	-1.443419000	2.685209000	1.084135000

O	-2.038217000	2.167180000	2.192448000
H	-0.352241000	2.819147000	1.177154000
C	-2.020573000	4.025115000	0.739197000
C	-3.166402000	4.651473000	1.111638000
O	-1.304640000	4.839741000	-0.080917000
C	-3.162305000	5.927367000	0.468620000
H	-3.919172000	4.247110000	1.769030000
C	-2.011393000	5.985863000	-0.241352000
H	-3.913709000	6.699771000	0.531936000
H	-1.562258000	6.738168000	-0.869970000
H	-1.086192000	1.804031000	3.355424000
O	-0.482727000	1.565073000	4.134590000
C	-0.736286000	2.461688000	5.183270000
H	-0.551280000	3.506396000	4.895924000
H	-1.770234000	2.395795000	5.550936000
H	-0.072207000	2.226027000	6.019934000
H	-4.958100000	-3.858373000	-0.729526000
H	6.630317000	-1.078572000	0.368699000
C	-0.904377000	-2.554577000	-3.543653000
H	-0.360691000	-2.183327000	-4.416802000
H	-0.191353000	-3.054812000	-2.884275000
H	-1.627208000	-3.299355000	-3.888959000
C	-2.562149000	-0.681487000	-3.777620000
H	-3.065630000	0.150051000	-3.279484000
H	-2.007798000	-0.280073000	-4.629864000
H	-3.326214000	-1.358431000	-4.168722000
C	2.681765000	-2.362910000	3.302311000
H	3.707537000	-2.622984000	3.577927000
H	2.064819000	-2.428231000	4.202396000
H	2.323229000	-3.107834000	2.588038000
C	3.067124000	0.084568000	3.737936000
H	4.102883000	-0.085766000	4.043555000
H	2.995043000	1.097399000	3.334490000
H	2.441700000	0.029500000	4.632518000
C	3.193592000	-1.406186000	-3.316103000
H	2.682769000	-1.214961000	-4.263514000
H	4.261022000	-1.511947000	-3.527507000
H	2.830699000	-2.357230000	-2.919079000
C	3.405912000	1.069612000	-2.916742000
H	2.905233000	1.267967000	-3.868128000
H	3.187630000	1.897315000	-2.237453000
H	4.483707000	1.058076000	-3.100990000
C	-3.122400000	-1.345937000	3.178172000
H	-2.700729000	-1.070200000	4.148201000
H	-3.634907000	-0.471960000	2.770937000
H	-3.867692000	-2.126160000	3.352706000

C	-1.329127000	-3.065732000	2.831960000
H	-2.040724000	-3.891536000	2.923763000
H	-0.502508000	-3.397469000	2.199935000
H	-0.933552000	-2.848393000	3.827984000

IPr-V-B Etot = -1960.457695544331 a.u.

C	0.385350000	-1.743165000	-0.193052000
C	-0.777925000	0.239406000	-0.161193000
C	0.537169000	0.512204000	0.017428000
H	1.050230000	1.450875000	0.146523000
N	-0.837818000	-1.150034000	-0.286895000
N	1.213783000	-0.689311000	-0.010626000
C	2.630046000	-0.799723000	0.134628000
C	3.432260000	-0.749472000	-1.012105000
C	3.172027000	-0.936559000	1.418280000
C	4.811298000	-0.846786000	-0.845624000
C	4.556835000	-1.027551000	1.533006000
C	5.370867000	-0.983670000	0.413606000
H	5.456283000	-0.812490000	-1.717029000
H	5.003534000	-1.135139000	2.515537000
C	-1.994817000	-1.982476000	-0.462284000
C	-2.614183000	-2.525436000	0.670563000
C	-2.401833000	-2.317026000	-1.757779000
C	-3.671181000	-3.408740000	0.476957000
C	-3.466302000	-3.204981000	-1.900731000
C	-4.099158000	-3.747269000	-0.796633000
H	-4.165457000	-3.843397000	1.338967000
H	-3.797132000	-3.480988000	-2.896064000
C	-1.712178000	-1.781761000	-2.993564000
H	-1.004719000	-1.012988000	-2.677858000
C	-2.158409000	-2.204308000	2.077192000
H	-1.447542000	-1.377637000	2.017439000
C	2.853600000	-0.591167000	-2.401177000
H	1.766608000	-0.547597000	-2.309481000
C	2.310223000	-0.983154000	2.660900000
H	1.265510000	-0.941603000	2.346492000
C	-1.956113000	1.208491000	-0.262432000
O	-3.136538000	0.622464000	0.053187000
H	-2.873079000	1.127463000	1.608645000
C	-1.924749000	1.825112000	-1.642529000
C	-0.962646000	1.973955000	-2.593061000
O	-3.068406000	2.418388000	-2.066880000
C	-1.553249000	2.710588000	-3.663850000
H	0.047222000	1.600556000	-2.539184000
C	-2.831217000	2.950633000	-3.288886000

H	-1.089532000	3.011052000	-4.591070000
H	-3.663535000	3.449906000	-3.758893000
C	-1.708833000	2.339326000	0.860715000
O	-2.230887000	1.773379000	2.029233000
H	-0.635624000	2.520059000	0.968305000
C	-2.376676000	3.641013000	0.582082000
C	-3.559508000	4.177626000	0.978193000
O	-1.721443000	4.520292000	-0.219257000
C	-3.643229000	5.467621000	0.369552000
H	-4.280666000	3.709073000	1.628672000
C	-2.504050000	5.620749000	-0.344825000
H	-4.443515000	6.186401000	0.458189000
H	-2.110505000	6.416553000	-0.956642000
O	-5.430956000	0.200166000	-1.080729000
C	-6.340143000	1.181780000	-0.657153000
H	-6.413652000	1.239246000	0.437824000
H	-6.078644000	2.182755000	-1.027622000
H	-7.331912000	0.932262000	-1.044357000
H	-4.526647000	0.424883000	-0.713817000
C	2.571381000	0.223811000	3.560602000
H	3.602298000	0.228012000	3.925343000
H	2.397329000	1.161251000	3.026771000
H	1.908153000	0.197838000	4.429218000
C	2.505953000	-2.288774000	3.428779000
H	3.530727000	-2.383110000	3.797861000
H	1.835686000	-2.321635000	4.291715000
H	2.291385000	-3.154776000	2.798056000
C	-0.919004000	-2.884957000	-3.693589000
H	-0.388967000	-2.481354000	-4.560843000
H	-0.183118000	-3.331738000	-3.020965000
H	-1.583678000	-3.679337000	-4.045289000
C	-2.695795000	-1.128374000	-3.961210000
H	-3.261507000	-0.331289000	-3.473611000
H	-2.156243000	-0.693422000	-4.806599000
H	-3.407515000	-1.855338000	-4.361389000
C	-1.435283000	-3.398965000	2.699141000
H	-2.109036000	-4.256391000	2.786408000
H	-0.577123000	-3.701291000	2.094758000
H	-1.077111000	-3.148654000	3.701689000
C	-3.311741000	-1.754096000	2.970992000
H	-2.928709000	-1.441043000	3.945903000
H	-3.851196000	-0.913949000	2.528630000
H	-4.026126000	-2.563551000	3.142685000
C	3.315951000	0.712677000	-3.049267000
H	2.852181000	0.830817000	-4.032143000
H	3.044693000	1.577297000	-2.438509000

H	4.400645000	0.722469000	-3.187085000
C	3.190539000	-1.790219000	-3.285528000
H	2.723000000	-1.677390000	-4.267233000
H	4.269576000	-1.880277000	-3.437158000
H	2.831457000	-2.721943000	-2.841935000
H	-4.924478000	-4.439059000	-0.927189000
H	6.447549000	-1.056487000	0.523268000

VI...IPr-I(H)-B Etot = -1960.444037547347 a.u.

C	0.473808000	-2.313209000	0.587756000
C	-0.479199000	-0.246326000	0.323749000
C	0.782165000	-0.176855000	-0.154538000
H	1.327587000	0.641518000	-0.595792000
N	-0.635789000	-1.548946000	0.764506000
N	1.335461000	-1.433516000	0.015835000
C	2.664863000	-1.772007000	-0.381829000
C	2.882925000	-2.229234000	-1.686974000
C	3.705878000	-1.627544000	0.542865000
C	4.187056000	-2.552975000	-2.052222000
C	4.992139000	-1.966027000	0.130563000
C	5.233068000	-2.424411000	-1.153844000
H	4.384773000	-2.912263000	-3.056395000
H	5.817416000	-1.868355000	0.827617000
C	-1.849133000	-2.039343000	1.337648000
C	-2.797647000	-2.640208000	0.501231000
C	-2.055407000	-1.890478000	2.714163000
C	-3.975519000	-3.102873000	1.082263000
C	-3.249096000	-2.369122000	3.247972000
C	-4.201480000	-2.970094000	2.442137000
H	-4.727500000	-3.573901000	0.458359000
H	-3.434071000	-2.269369000	4.312112000
C	-1.032603000	-1.242062000	3.621472000
H	-0.190543000	-0.922116000	3.004503000
C	-2.581462000	-2.797695000	-0.988210000
H	-1.605956000	-2.372854000	-1.232217000
C	1.760639000	-2.383759000	-2.690106000
H	0.831754000	-2.075257000	-2.206458000
C	3.474469000	-1.127347000	1.951941000
H	2.410673000	-0.906592000	2.059763000
C	-2.557464000	3.299646000	-1.341123000
O	-2.041899000	2.432465000	-2.033921000
H	-1.270263000	0.501833000	0.384078000
C	-2.512949000	4.693773000	-1.753639000
C	-2.880959000	5.867869000	-1.154314000
O	-1.993016000	4.964318000	-2.985638000

C	-2.574144000	6.905618000	-2.066591000
H	-3.316350000	5.973832000	-0.173761000
C	-2.039292000	6.292510000	-3.156581000
H	-2.724835000	7.965470000	-1.935110000
H	-1.660343000	6.665431000	-4.095558000
C	-3.255680000	2.943217000	0.000285000
O	-2.699160000	1.896785000	0.623052000
H	-3.238034000	3.890580000	0.587801000
C	-4.717779000	2.720698000	-0.347969000
C	-5.480475000	1.597567000	-0.333022000
O	-5.479845000	3.782448000	-0.728650000
C	-6.795817000	1.991936000	-0.731350000
H	-5.139751000	0.612423000	-0.058404000
C	-6.736906000	3.324463000	-0.958448000
H	-7.669274000	1.365283000	-0.829849000
H	-7.462302000	4.060020000	-1.267766000
O	-0.439155000	2.207987000	-4.300404000
C	-1.109147000	1.215045000	-5.045664000
H	-1.270244000	0.300061000	-4.462437000
H	-2.081514000	1.562590000	-5.416082000
H	-0.487873000	0.963225000	-5.907367000
H	-0.985894000	2.409224000	-3.519360000
H	-5.125602000	-3.336235000	2.876309000
H	6.242124000	-2.682598000	-1.456672000
C	-3.631146000	-2.029667000	-1.788967000
H	-3.629018000	-0.968825000	-1.527547000
H	-3.426748000	-2.117884000	-2.859332000
H	-4.635365000	-2.421838000	-1.606244000
C	-2.553400000	-4.270392000	-1.392743000
H	-2.352206000	-4.363615000	-2.463288000
H	-1.776270000	-4.814718000	-0.850714000
H	-3.512063000	-4.755070000	-1.188692000
C	1.969345000	-1.481563000	-3.904998000
H	2.049469000	-0.432135000	-3.611028000
H	2.878992000	-1.752127000	-4.448021000
H	1.126601000	-1.578052000	-4.594562000
C	1.592380000	-3.841918000	-3.113711000
H	0.747996000	-3.939599000	-3.801193000
H	2.485427000	-4.211097000	-3.625303000
H	1.405598000	-4.485109000	-2.250359000
C	4.243442000	0.165286000	2.218825000
H	4.022671000	0.533994000	3.223950000
H	5.322996000	0.005942000	2.150862000
H	3.970569000	0.944086000	1.502583000
C	3.827364000	-2.196422000	2.984601000
H	3.253490000	-3.111279000	2.818428000

H	4.890137000	-2.450421000	2.943078000
H	3.608372000	-1.834111000	3.992550000
C	-1.599894000	-0.000128000	4.306537000
H	-1.957979000	0.727751000	3.574485000
H	-2.434336000	-0.256708000	4.964824000
H	-0.828934000	0.478969000	4.915770000
C	-0.495586000	-2.237157000	4.648866000
H	-1.290402000	-2.585932000	5.313920000
H	-0.054945000	-3.109892000	4.160778000
H	0.274577000	-1.765503000	5.265010000

IPr-TS1^{Ph}-A $i137\text{ cm}^{-1}$ Etot= -1620.005524787156

H	-1.359985000000	4.093170000000	0.262833000000
C	-2.226554000000	2.171101000000	0.925312000000
C	-1.377304000000	3.017339000000	0.309707000000
N	-1.777972000000	0.895291000000	0.638486000000
C	-0.667888000000	0.913008000000	-0.133370000000
N	-0.433568000000	2.231506000000	-0.326209000000
H	-3.099615000000	2.355719000000	1.528733000000
H	2.875593000000	-0.739976000000	1.215896000000
O	3.410624000000	-1.048269000000	1.979212000000
C	0.811408000000	-0.803589000000	-0.347581000000
O	1.948795000000	-0.333312000000	-0.195908000000
C	0.646143000000	2.778760000000	-1.098810000000
C	1.778498000000	3.259089000000	-0.428675000000
C	0.507053000000	2.854500000000	-2.493757000000
C	2.795678000000	3.818274000000	-1.199111000000
C	1.558788000000	3.411462000000	-3.214341000000
C	2.691050000000	3.890170000000	-2.575604000000
H	3.684566000000	4.200704000000	-0.710752000000
H	1.489746000000	3.479473000000	-4.293052000000
C	-2.444708000000	-0.287728000000	1.100752000000
C	-3.497298000000	-0.805123000000	0.334066000000
C	-2.053742000000	-0.851653000000	2.321367000000
C	-4.152219000000	-1.934208000000	0.817497000000
C	-2.742925000000	-1.979575000000	2.759750000000
C	-3.778880000000	-2.517742000000	2.016207000000
H	-4.971581000000	-2.359798000000	0.249849000000
H	-2.466989000000	-2.439368000000	3.701600000000
C	1.913511000000	3.220787000000	1.078798000000
H	1.150833000000	2.542605000000	1.468178000000
C	-0.963389000000	-0.246539000000	3.178027000000
H	-0.385057000000	0.436582000000	2.550766000000
C	-3.965916000000	-0.145523000000	-0.944771000000
H	-3.183278000000	0.539069000000	-1.277951000000

C	-0.758228000000	2.412261000000	-3.198953000000
H	-1.186864000000	1.587578000000	-2.622644000000
H	0.267852000000	-1.229372000000	0.508254000000
C	4.325763000000	-2.013417000000	1.514172000000
H	5.025720000000	-1.599630000000	0.777375000000
H	4.905913000000	-2.370974000000	2.367504000000
H	3.822375000000	-2.876446000000	1.060665000000
H	3.496806000000	4.324416000000	-3.157517000000
H	-4.302777000000	-3.396692000000	2.375881000000
C	3.270400000000	2.690287000000	1.533213000000
H	3.285282000000	2.602111000000	2.622587000000
H	3.475549000000	1.705989000000	1.110262000000
H	4.082171000000	3.364330000000	1.248765000000
C	1.662846000000	4.606328000000	1.677318000000
H	0.686219000000	5.002645000000	1.391834000000
H	1.705926000000	4.559842000000	2.768612000000
H	2.425414000000	5.313464000000	1.338343000000
C	-1.574578000000	0.571315000000	4.317509000000
H	-2.242638000000	1.349240000000	3.940654000000
H	-2.149736000000	-0.073703000000	4.987798000000
H	-0.786601000000	1.052255000000	4.902566000000
C	0.002519000000	-1.288783000000	3.734220000000
H	-0.493892000000	-1.961321000000	4.438085000000
H	0.447272000000	-1.895717000000	2.942522000000
H	0.812037000000	-0.789605000000	4.272188000000
C	-5.228449000000	0.678982000000	-0.683534000000
H	-5.539951000000	1.193277000000	-1.596545000000
H	-6.049379000000	0.031558000000	-0.362220000000
H	-5.067136000000	1.429922000000	0.092933000000
C	-4.207390000000	-1.142407000000	-2.073789000000
H	-3.317545000000	-1.744450000000	-2.269174000000
H	-5.037293000000	-1.816782000000	-1.848526000000
H	-4.463318000000	-0.604399000000	-2.990136000000
C	-0.522634000000	1.903838000000	-4.615952000000
H	-0.216845000000	2.708107000000	-5.289982000000
H	0.237591000000	1.120494000000	-4.645725000000
H	-1.452447000000	1.486250000000	-5.009861000000
C	-1.779150000000	3.554062000000	-3.223041000000
H	-1.399304000000	4.388253000000	-3.820096000000
H	-2.716637000000	3.215512000000	-3.671978000000
H	-1.999401000000	3.927682000000	-2.221621000000
C	0.381755000000	-1.365080000000	-1.659694000000
C	1.023258000000	-0.992337000000	-2.837943000000
C	-0.595843000000	-2.353770000000	-1.696533000000
C	0.679234000000	-1.590640000000	-4.038927000000
C	-0.934127000000	-2.962117000000	-2.897725000000

C	-0.298966000000	-2.578895000000	-4.071541000000
H	1.790851000000	-0.227845000000	-2.796735000000
H	-1.091709000000	-2.649221000000	-0.776964000000
H	1.172902000000	-1.284329000000	-4.954731000000
H	-1.694713000000	-3.734830000000	-2.920308000000
H	-0.563327000000	-3.051046000000	-5.011302000000

IPr-II^{Ph}-A

Etot = -1620.035617342329

C	-0.285088000000	-0.268107000000	-0.023228000000
C	-1.041587000000	-2.279756000000	-0.597106000000
H	-1.770797000000	-3.063092000000	-0.709484000000
C	0.263949000000	-2.230798000000	-0.924531000000
H	0.911245000000	-2.962397000000	-1.376632000000
N	-1.369458000000	-1.062218000000	-0.038259000000
N	0.717756000000	-0.982008000000	-0.565055000000
C	2.063325000000	-0.535114000000	-0.812154000000
C	3.018921000000	-0.687949000000	0.199878000000
C	2.368511000000	-0.032410000000	-2.082654000000
C	4.319213000000	-0.283859000000	-0.086752000000
C	3.685836000000	0.354937000000	-2.313037000000
C	4.649322000000	0.235704000000	-1.327033000000
H	5.087064000000	-0.383736000000	0.670937000000
H	3.961462000000	0.749082000000	-3.284083000000
C	-2.701008000000	-0.782684000000	0.437051000000
C	-3.058708000000	-1.244207000000	1.709606000000
C	-3.603405000000	-0.158699000000	-0.432773000000
C	-4.367578000000	-1.014791000000	2.124150000000
C	-4.897594000000	0.046069000000	0.036512000000
C	-5.274818000000	-0.369605000000	1.302085000000
H	-4.681623000000	-1.352107000000	3.104708000000
H	-5.625031000000	0.530752000000	-0.603319000000
C	-3.232030000000	0.217456000000	-1.850712000000
H	-2.149752000000	0.359283000000	-1.883636000000
C	-2.108817000000	-2.018007000000	2.599087000000
H	-1.088343000000	-1.832973000000	2.252506000000
C	2.694727000000	-1.320816000000	1.535535000000
H	1.613245000000	-1.267290000000	1.686213000000
C	1.352364000000	0.038048000000	-3.202623000000
H	0.356688000000	-0.066023000000	-2.765733000000
C	-0.153247000000	1.210396000000	0.312889000000
O	-0.578826000000	1.919756000000	-0.759697000000
H	0.379179000000	3.084798000000	-0.998553000000
H	0.937643000000	1.316741000000	0.494400000000
O	1.045415000000	3.841042000000	-1.166017000000
C	0.712923000000	4.924256000000	-0.340966000000

H	0.738450000000	4.663819000000	0.727056000000
H	1.436202000000	5.729600000000	-0.500935000000
H	-0.286341000000	5.328548000000	-0.559073000000
C	-0.794029000000	1.606883000000	1.645009000000
C	-1.976380000000	2.336826000000	1.663345000000
C	-0.143538000000	1.358466000000	2.850133000000
C	-2.508504000000	2.795036000000	2.861214000000
C	-0.664352000000	1.823586000000	4.049999000000
C	-1.852465000000	2.542909000000	4.059578000000
H	-2.462900000000	2.556163000000	0.720548000000
H	0.794792000000	0.812894000000	2.849172000000
H	-3.432889000000	3.363116000000	2.858572000000
H	-0.137566000000	1.630603000000	4.978482000000
H	-2.259822000000	2.912358000000	4.994324000000
H	5.669295000000	0.544156000000	-1.528455000000
H	-6.289154000000	-0.199367000000	1.646217000000
C	3.355508000000	-0.602866000000	2.708358000000
H	2.987340000000	-1.019267000000	3.648879000000
H	4.440705000000	-0.729064000000	2.698090000000
H	3.139416000000	0.467799000000	2.700251000000
C	3.087079000000	-2.800057000000	1.527934000000
H	2.818374000000	-3.266649000000	2.479093000000
H	2.586861000000	-3.347185000000	0.725924000000
H	4.166488000000	-2.907524000000	1.389317000000
C	-2.179429000000	-1.588256000000	4.061220000000
H	-3.139059000000	-1.853817000000	4.511280000000
H	-1.399649000000	-2.100293000000	4.630486000000
H	-2.032318000000	-0.513153000000	4.171165000000
C	-2.381890000000	-3.520486000000	2.488937000000
H	-2.307398000000	-3.879423000000	1.460930000000
H	-1.665481000000	-4.078043000000	3.097601000000
H	-3.387190000000	-3.749895000000	2.853241000000
C	-3.613599000000	-0.910390000000	-2.812365000000
H	-3.305937000000	-0.657202000000	-3.830404000000
H	-3.140370000000	-1.856482000000	-2.541037000000
H	-4.696727000000	-1.063762000000	-2.813925000000
C	-3.859623000000	1.530494000000	-2.306039000000
H	-3.461311000000	1.803674000000	-3.286230000000
H	-4.945057000000	1.452137000000	-2.406539000000
H	-3.636897000000	2.342829000000	-1.611008000000
C	1.564028000000	-1.118578000000	-4.181725000000
H	2.544952000000	-1.042757000000	-4.659319000000
H	1.506252000000	-2.088585000000	-3.683046000000
H	0.802703000000	-1.092122000000	-4.965593000000
C	1.381452000000	1.372490000000	-3.942143000000
H	2.319984000000	1.512538000000	-4.484229000000

H	0.572743000000	1.400752000000	-4.676746000000
H	1.251328000000	2.211811000000	-3.256734000000

IPr-TS2^{Ph}-A i 1191 cm⁻¹ Etot = -1619.995578804062

C	-0.366954000000	-0.128151000000	-0.004324000000
C	-1.162862000000	-2.110298000000	-0.687137000000
H	-1.920359000000	-2.839541000000	-0.916614000000
C	0.174347000000	-2.172066000000	-0.754305000000
H	0.834533000000	-2.962395000000	-1.066183000000
N	-1.496644000000	-0.850183000000	-0.223651000000
N	0.664180000000	-0.951002000000	-0.330559000000
C	2.077679000000	-0.692755000000	-0.312798000000
C	2.823660000000	-1.143586000000	0.783304000000
C	2.664902000000	-0.108194000000	-1.441937000000
C	4.201553000000	-0.951098000000	0.741806000000
C	4.045640000000	0.064145000000	-1.428017000000
C	4.806248000000	-0.346447000000	-0.346478000000
H	4.811262000000	-1.285396000000	1.572923000000
H	4.534988000000	0.516435000000	-2.282227000000
C	-2.883760000000	-0.518741000000	-0.020047000000
C	-3.446215000000	-0.734549000000	1.242864000000
C	-3.640093000000	-0.122267000000	-1.127008000000
C	-4.811907000000	-0.512785000000	1.383738000000
C	-5.003339000000	0.086817000000	-0.930784000000
C	-5.585120000000	-0.102373000000	0.310001000000
H	-5.279660000000	-0.668738000000	2.348968000000
H	-5.618911000000	0.395878000000	-1.767863000000
C	-3.048266000000	0.044423000000	-2.510707000000
H	-1.959371000000	0.009924000000	-2.423503000000
C	-2.632986000000	-1.226553000000	2.420142000000
H	-1.575330000000	-1.083005000000	2.186374000000
C	2.195736000000	-1.867066000000	1.955461000000
H	1.120897000000	-1.667253000000	1.940803000000
C	1.863914000000	0.262893000000	-2.671716000000
H	0.819315000000	0.383801000000	-2.374882000000
C	-0.294411000000	1.282254000000	0.357200000000
O	-1.572552000000	1.758452000000	0.755902000000
H	-1.777144000000	2.408211000000	0.058852000000
H	-0.206579000000	2.031935000000	-0.714056000000
O	-0.669709000000	2.949034000000	-1.524091000000
C	-0.149861000000	4.210808000000	-1.273477000000
H	-0.109689000000	4.458104000000	-0.197827000000
H	0.878106000000	4.340160000000	-1.658149000000
H	-0.760792000000	4.996048000000	-1.748393000000
C	-2.859788000000	-2.723250000000	2.640813000000

H	-2.238803000000	-3.083379000000	3.465296000000
H	-3.905709000000	-2.919725000000	2.893125000000
H	-2.612629000000	-3.303433000000	1.748906000000
C	-2.923355000000	-0.448684000000	3.700551000000
H	-2.236492000000	-0.765790000000	4.489203000000
H	-2.801258000000	0.626570000000	3.552615000000
H	-3.939606000000	-0.628520000000	4.059704000000
C	-3.410292000000	1.387345000000	-3.140045000000
H	-4.488257000000	1.482905000000	-3.290935000000
H	-3.064783000000	2.217553000000	-2.521679000000
H	-2.931764000000	1.475155000000	-4.118959000000
C	-3.480424000000	-1.105996000000	-3.421563000000
H	-4.565454000000	-1.101719000000	-3.558679000000
H	-3.015471000000	-1.003383000000	-4.405495000000
H	-3.196724000000	-2.076949000000	-3.009363000000
C	2.310404000000	1.576905000000	-3.304811000000
H	2.311232000000	2.394706000000	-2.581234000000
H	3.311847000000	1.499165000000	-3.734794000000
H	1.626822000000	1.842870000000	-4.114493000000
C	2.396985000000	-3.378566000000	1.820817000000
H	1.907591000000	-3.898208000000	2.648630000000
H	1.987654000000	-3.766601000000	0.886339000000
H	3.462424000000	-3.623868000000	1.849779000000
C	2.731997000000	-1.392346000000	3.302649000000
H	2.639684000000	-0.311043000000	3.412760000000
H	2.167478000000	-1.867498000000	4.108878000000
H	3.781818000000	-1.664983000000	3.435589000000
H	-6.648824000000	0.063782000000	0.440929000000
H	5.881453000000	-0.204678000000	-0.357553000000
C	1.929533000000	-0.866964000000	-3.702355000000
H	2.958804000000	-1.013752000000	-4.041847000000
H	1.571250000000	-1.813154000000	-3.291491000000
H	1.316678000000	-0.619231000000	-4.572939000000
C	0.756444000000	1.710788000000	1.352022000000
C	0.503424000000	1.611941000000	2.721244000000
C	1.933271000000	2.333082000000	0.944558000000
C	1.398541000000	2.117837000000	3.652237000000
C	2.841005000000	2.827419000000	1.872558000000
C	2.575089000000	2.725386000000	3.230913000000
H	-0.416488000000	1.148723000000	3.059433000000
H	2.135446000000	2.444461000000	-0.114074000000
H	1.179236000000	2.034139000000	4.711428000000
H	3.750492000000	3.309830000000	1.530796000000
H	3.276387000000	3.121488000000	3.957131000000

IPr-III^{Ph}-A

Etot = -1620.022258285446

C	-0.271612000000	-0.283316000000	-0.054082000000
C	-1.123489000000	-2.157584000000	-1.003078000000
H	-1.892100000000	-2.844845000000	-1.312984000000
C	0.201026000000	-2.193808000000	-1.178811000000
H	0.826201000000	-2.941399000000	-1.633981000000
N	-1.432620000000	-0.990463000000	-0.316829000000
N	0.747968000000	-1.051191000000	-0.598035000000
C	2.146694000000	-0.962113000000	-0.325288000000
C	3.030551000000	-0.719719000000	-1.390123000000
C	2.608776000000	-1.206590000000	0.976711000000
C	4.393148000000	-0.675064000000	-1.109383000000
C	3.979372000000	-1.126211000000	1.206684000000
C	4.865854000000	-0.856037000000	0.178417000000
H	5.095382000000	-0.493227000000	-1.914977000000
H	4.360215000000	-1.307964000000	2.205617000000
C	-2.772356000000	-0.503343000000	-0.233297000000
C	-3.624191000000	-1.035527000000	0.744257000000
C	-3.215971000000	0.436780000000	-1.172683000000
C	-4.942559000000	-0.591931000000	0.771618000000
C	-4.539897000000	0.862423000000	-1.091697000000
C	-5.397454000000	0.355089000000	-0.131157000000
H	-5.623646000000	-0.991151000000	1.515033000000
H	-4.907202000000	1.592669000000	-1.804677000000
C	-2.331263000000	0.974816000000	-2.276596000000
H	-1.342736000000	0.523748000000	-2.173428000000
C	-3.157337000000	-2.074168000000	1.740437000000
H	-2.070379000000	-2.147320000000	1.657549000000
C	2.562793000000	-0.562788000000	-2.823387000000
H	1.479169000000	-0.417962000000	-2.809648000000
C	1.699815000000	-1.647517000000	2.104294000000
H	0.665739000000	-1.544807000000	1.774471000000
C	-0.200892000000	0.889130000000	0.676167000000
O	-1.273031000000	1.089146000000	1.556797000000
H	-1.193412000000	1.095412000000	3.412044000000
O	-1.210339000000	1.161871000000	4.382870000000
C	-2.204056000000	2.098962000000	4.740027000000
H	-2.206505000000	2.186327000000	5.827850000000
H	-2.004104000000	3.090936000000	4.317335000000
H	-3.203556000000	1.780613000000	4.419616000000
H	-1.797169000000	1.845572000000	1.264240000000
H	-6.427094000000	0.693613000000	-0.089778000000
H	5.930735000000	-0.806518000000	0.378245000000
C	1.935677000000	-3.125716000000	2.420310000000
H	1.243934000000	-3.459664000000	3.198317000000
H	1.783242000000	-3.750547000000	1.536884000000

H	2.954834000000	-3.291054000000	2.780531000000
C	1.864663000000	-0.793879000000	3.358018000000
H	1.690090000000	0.262475000000	3.143486000000
H	1.148881000000	-1.109592000000	4.121233000000
H	2.866614000000	-0.896084000000	3.782999000000
C	-3.482929000000	-1.682648000000	3.179624000000
H	-4.561797000000	-1.647053000000	3.351212000000
H	-3.063925000000	-2.420499000000	3.868852000000
H	-3.064202000000	-0.706434000000	3.432172000000
C	-3.746448000000	-3.447071000000	1.414522000000
H	-3.491229000000	-3.765609000000	0.401311000000
H	-3.367921000000	-4.197684000000	2.113446000000
H	-4.836991000000	-3.428618000000	1.496996000000
C	-2.869705000000	0.582902000000	-3.652221000000
H	-2.965281000000	-0.501519000000	-3.746380000000
H	-3.852238000000	1.026759000000	-3.833733000000
H	-2.193116000000	0.935270000000	-4.435232000000
C	-2.157992000000	2.488497000000	-2.171464000000
H	-1.476926000000	2.845053000000	-2.948660000000
H	-3.112672000000	3.005432000000	-2.300949000000
H	-1.745062000000	2.773352000000	-1.200837000000
C	2.860434000000	-1.830322000000	-3.628732000000
H	2.471510000000	-1.731451000000	-4.645529000000
H	3.939821000000	-1.993662000000	-3.694784000000
H	2.415847000000	-2.720247000000	-3.179710000000
C	3.183783000000	0.640744000000	-3.529873000000
H	3.007119000000	1.571986000000	-2.989490000000
H	4.263053000000	0.520322000000	-3.650881000000
H	2.751663000000	0.742658000000	-4.528479000000
C	0.807274000000	1.915494000000	0.651240000000
C	0.936895000000	2.814270000000	1.730394000000
C	1.636471000000	2.146059000000	-0.462890000000
C	1.859988000000	3.846946000000	1.705690000000
C	2.563122000000	3.172934000000	-0.476887000000
C	2.692288000000	4.034465000000	0.608606000000
H	0.308162000000	2.687866000000	2.603262000000
H	1.515542000000	1.529398000000	-1.343668000000
H	1.931885000000	4.512210000000	2.560420000000
H	3.179783000000	3.319481000000	-1.358265000000
H	3.413834000000	4.843147000000	0.590817000000

IPr-TS1^{Ph}-B $i221\text{ cm}^{-1}$ Etot = -1619.491471909139

C	-0.083486000000	-2.708396000000	-0.910252000000
C	-1.452367000000	-0.943638000000	-1.356157000000
H	-2.394177000000	-0.418474000000	-1.374679000000

C	-0.222777000000	-0.566899000000	-1.783448000000
H	2.687042000000	1.767200000000	-2.711834000000
N	-1.347618000000	-2.230024000000	-0.839079000000
N	0.581589000000	-1.666193000000	-1.489505000000
C	1.981898000000	-1.736869000000	-1.762788000000
C	2.892575000000	-1.405295000000	-0.749930000000
C	2.408417000000	-2.160957000000	-3.027405000000
C	4.251955000000	-1.506655000000	-1.032845000000
C	3.778833000000	-2.239164000000	-3.265999000000
C	4.695208000000	-1.916547000000	-2.279501000000
H	4.975950000000	-1.263243000000	-0.262901000000
H	4.132058000000	-2.566830000000	-4.238074000000
C	-2.445814000000	-2.950984000000	-0.287412000000
C	-3.196692000000	-3.792192000000	-1.118387000000
C	-2.756161000000	-2.778061000000	1.067473000000
C	-4.273454000000	-4.473409000000	-0.556574000000
C	-3.842791000000	-3.479308000000	1.583732000000
C	-4.596227000000	-4.320482000000	0.781686000000
H	-4.868043000000	-5.134273000000	-1.178279000000
H	-4.101591000000	-3.365256000000	2.631068000000
C	-1.949712000000	-1.867662000000	1.967903000000
H	-1.150028000000	-1.429223000000	1.367668000000
C	-2.871274000000	-3.978456000000	-2.584098000000
H	-2.002068000000	-3.358760000000	-2.813138000000
C	2.442864000000	-0.983055000000	0.632495000000
H	1.365689000000	-0.808519000000	0.591033000000
C	1.435699000000	-2.567812000000	-4.113802000000
H	0.424973000000	-2.429552000000	-3.724748000000
O	3.519314000000	1.758279000000	-3.270041000000
C	4.532723000000	2.421521000000	-2.560451000000
H	5.426087000000	2.471180000000	-3.188717000000
H	4.252286000000	3.450177000000	-2.295190000000
H	4.804532000000	1.896420000000	-1.633826000000
C	0.365411000000	1.290027000000	-2.552535000000
H	0.600487000000	0.883946000000	-3.549118000000
O	1.314052000000	1.820721000000	-1.882875000000
H	-5.439031000000	-4.859159000000	1.201428000000
H	5.758694000000	-1.986852000000	-2.481563000000
C	-2.497883000000	-5.427778000000	-2.890153000000
H	-3.340708000000	-6.099770000000	-2.706019000000
H	-2.210727000000	-5.530957000000	-3.940043000000
H	-1.659896000000	-5.759617000000	-2.272511000000
C	-4.021373000000	-3.513348000000	-3.475523000000
H	-3.742377000000	-3.603118000000	-4.528781000000
H	-4.917644000000	-4.118793000000	-3.314451000000
H	-4.278810000000	-2.469682000000	-3.278965000000

C	1.596914000000	-4.045990000000	-4.467029000000
H	0.842623000000	-4.344701000000	-5.200021000000
H	2.581516000000	-4.243860000000	-4.899856000000
H	1.483857000000	-4.678225000000	-3.583020000000
C	1.576120000000	-1.696205000000	-5.360221000000
H	2.586361000000	-1.749952000000	-5.774315000000
H	0.879327000000	-2.031732000000	-6.133336000000
H	1.352808000000	-0.650515000000	-5.138503000000
C	3.104107000000	0.315092000000	1.089582000000
H	2.695477000000	0.620291000000	2.056657000000
H	4.183944000000	0.196317000000	1.211866000000
H	2.928585000000	1.121958000000	0.374785000000
C	2.692545000000	-2.100352000000	1.645459000000
H	2.177862000000	-3.018995000000	1.354566000000
H	3.761378000000	-2.319411000000	1.725891000000
H	2.333738000000	-1.804717000000	2.635327000000
C	-1.294896000000	-2.648949000000	3.105506000000
H	-2.045660000000	-3.102696000000	3.758371000000
H	-0.654724000000	-3.446140000000	2.719795000000
H	-0.679604000000	-1.982568000000	3.715930000000
C	-2.801392000000	-0.721437000000	2.511205000000
H	-3.242865000000	-0.136197000000	1.700187000000
H	-3.614145000000	-1.094987000000	3.140248000000
H	-2.188334000000	-0.051395000000	3.119792000000
C	-0.993592000000	1.924450000000	-2.533645000000
C	-1.909996000000	1.661871000000	-3.549410000000
C	-1.345184000000	2.821088000000	-1.529398000000
C	-3.158025000000	2.267253000000	-3.553770000000
C	-2.595235000000	3.425505000000	-1.526549000000
C	-3.507594000000	3.149694000000	-2.537403000000
H	-1.637207000000	0.973070000000	-4.343972000000
H	-0.623314000000	3.043787000000	-0.751576000000
H	-3.859817000000	2.054843000000	-4.353375000000
H	-2.857786000000	4.118391000000	-0.734056000000
H	-4.482606000000	3.624579000000	-2.538261000000

IPr-II^{Ph}-B

Etot = -1619.533936179433

C	-0.710146000	-0.676996000	0.690327000
C	0.474289000	-1.079606000	0.175667000
N	-1.688632000	-1.018686000	-0.225200000
C	-1.184213000	-1.639184000	-1.318814000
N	0.150602000	-1.658973000	-1.051471000
H	-0.937403000	-0.186198000	1.622311000
O	1.363324000	2.365000000	-0.158051000
C	1.890052000	-0.903292000	0.689975000

O	2.532268000	0.144468000	0.100270000
H	1.812776000	1.438386000	-0.032740000
C	2.333407000	3.359935000	0.000233000
H	2.826506000	3.315354000	0.983445000
H	3.123420000	3.307508000	-0.764511000
H	1.861860000	4.344594000	-0.084512000
H	2.400672000	-1.863909000	0.460984000
C	-3.076700000	-0.751486000	-0.026825000
C	-3.605030000	0.460786000	-0.487682000
C	-3.861542000	-1.701357000	0.638460000
C	-4.958674000	0.704779000	-0.270678000
C	-5.210062000	-1.411860000	0.830370000
C	-5.755864000	-0.220853000	0.381587000
H	-5.393857000	1.635725000	-0.617813000
H	-5.841473000	-2.131315000	1.340620000
C	1.083921000	-2.274478000	-1.943961000
C	1.531453000	-1.562716000	-3.065558000
C	1.491048000	-3.591859000	-1.692554000
C	2.405046000	-2.205458000	-3.939076000
C	2.370897000	-4.188095000	-2.592430000
C	2.825455000	-3.503901000	-3.706585000
H	2.759321000	-1.679604000	-4.818677000
H	2.695077000	-5.208987000	-2.423390000
C	1.070628000	-0.154336000	-3.373056000
H	0.558948000	0.228644000	-2.487913000
C	0.963424000	-4.393902000	-0.521975000
H	0.428675000	-3.711044000	0.141453000
C	-2.758865000	1.495480000	-1.196639000
H	-1.749176000	1.092470000	-1.295402000
C	-3.294009000	-3.008937000	1.146157000
H	-2.234347000	-3.038358000	0.884924000
H	3.506948000	-3.986119000	-4.399204000
H	-6.808321000	-0.012666000	0.541540000
C	2.234192000	0.786240000	-3.677578000
H	2.967136000	0.787049000	-2.868046000
H	2.747013000	0.507447000	-4.601740000
H	1.863116000	1.806864000	-3.802398000
C	0.068323000	-0.154538000	-4.527427000
H	0.533849000	-0.528127000	-5.444240000
H	-0.794707000	-0.784218000	-4.301507000
H	-0.288599000	0.860954000	-4.720432000
C	-3.280027000	1.774896000	-2.604838000
H	-3.320424000	0.859902000	-3.200702000
H	-4.284148000	2.206768000	-2.578402000
H	-2.624053000	2.485462000	-3.114595000
C	-2.664103000	2.785526000	-0.383531000

H	-3.646824000	3.250243000	-0.264352000
H	-2.254924000	2.597715000	0.612078000
H	-2.012215000	3.502845000	-0.889035000
C	-3.965316000	-4.205701000	0.475075000
H	-3.866573000	-4.156522000	-0.612005000
H	-3.505973000	-5.136736000	0.817611000
H	-5.030706000	-4.249411000	0.717171000
C	-3.397818000	-3.106835000	2.667208000
H	-4.441482000	-3.103893000	2.993515000
H	-2.940157000	-4.035840000	3.017348000
H	-2.888653000	-2.271442000	3.154034000
C	-0.037362000	-5.445158000	-1.003077000
H	-0.453364000	-5.991854000	-0.152380000
H	-0.862857000	-4.984617000	-1.550946000
H	0.447818000	-6.168219000	-1.665027000
C	2.079384000	-5.044178000	0.291449000
H	2.802036000	-4.302605000	0.640296000
H	1.658741000	-5.546452000	1.166493000
H	2.618361000	-5.795119000	-0.291844000
C	1.854407000	-0.842738000	2.221412000
C	1.485677000	-1.953349000	2.980360000
C	2.221488000	0.319237000	2.886997000
C	1.473731000	-1.900077000	4.365979000
C	2.207968000	0.381610000	4.277068000
C	1.833490000	-0.726894000	5.022432000
H	1.203710000	-2.873747000	2.476830000
H	2.527153000	1.173763000	2.294308000
H	1.187124000	-2.776263000	4.938386000
H	2.495165000	1.300142000	4.778748000
H	1.826165000	-0.682638000	6.106138000

IPr-TS2^{Ph}-B i 1156 cm⁻¹ Etot = -1619.490911017558

C	-0.400291000000	-0.882176000000	0.433198000000
C	0.741083000000	-1.119716000000	-0.263321000000
N	-1.464512000000	-1.208772000000	-0.381581000000
C	-1.066168000000	-1.648117000000	-1.600964000000
N	0.288488000000	-1.582748000000	-1.507222000000
H	-0.535768000000	-0.515911000000	1.437691000000
O	4.256624000000	-1.653424000000	-1.143227000000
C	2.148990000000	-0.887782000000	0.129022000000
O	2.547398000000	0.422611000000	-0.331173000000
H	3.374514000000	0.266458000000	-0.807892000000
C	5.212728000000	-2.202181000000	-0.295255000000
H	5.827569000000	-1.439088000000	0.213464000000
H	4.764258000000	-2.822010000000	0.498455000000

H	5.908156000000	-2.853371000000	-0.846849000000
H	3.227906000000	-1.547811000000	-0.561435000000
C	-2.829748000000	-1.102738000000	0.019970000000
C	-3.533753000000	0.072252000000	-0.271544000000
C	-3.419278000000	-2.172678000000	0.705052000000
C	-4.863831000000	0.151825000000	0.133477000000
C	-4.750220000000	-2.043661000000	1.093181000000
C	-5.468813000000	-0.894248000000	0.809592000000
H	-5.433113000000	1.049557000000	-0.082535000000
H	-5.231008000000	-2.858021000000	1.624383000000
C	1.114754000000	-2.047724000000	-2.577417000000
C	1.497746000000	-1.157715000000	-3.588456000000
C	1.468389000000	-3.402544000000	-2.610015000000
C	2.254248000000	-1.657889000000	-4.645346000000
C	2.225561000000	-3.855501000000	-3.687053000000
C	2.617198000000	-2.993340000000	-4.696968000000
H	2.558505000000	-0.991847000000	-5.445053000000
H	2.508279000000	-4.901576000000	-3.737108000000
C	1.078758000000	0.296234000000	-3.583291000000
H	0.703926000000	0.527458000000	-2.584542000000
C	1.037240000000	-4.380648000000	-1.538263000000
H	0.519033000000	-3.817965000000	-0.759305000000
C	-2.899382000000	1.238023000000	-0.997936000000
H	-1.860656000000	0.976089000000	-1.208062000000
C	-2.661178000000	-3.440918000000	1.030826000000
H	-1.662862000000	-3.355258000000	0.597167000000
H	3.205493000000	-3.363811000000	-5.529725000000
H	-6.505496000000	-0.812945000000	1.118305000000
C	0.052172000000	-5.406140000000	-2.098305000000
H	0.520905000000	-6.016046000000	-2.875824000000
H	-0.288741000000	-6.077334000000	-1.305251000000
H	-0.823575000000	-4.918076000000	-2.532557000000
C	2.229499000000	-5.077351000000	-0.886168000000
H	2.927903000000	-4.353836000000	-0.459876000000
H	1.885807000000	-5.734489000000	-0.082799000000
H	2.775655000000	-5.691871000000	-1.606948000000
C	-3.326594000000	-4.667491000000	0.410122000000
H	-3.421716000000	-4.560678000000	-0.673133000000
H	-2.731400000000	-5.561645000000	0.613480000000
H	-4.325378000000	-4.830591000000	0.823887000000
C	-2.497053000000	-3.614169000000	2.539938000000
H	-3.467939000000	-3.720994000000	3.031766000000
H	-1.910914000000	-4.511316000000	2.756202000000
H	-1.984952000000	-2.757141000000	2.984228000000
C	-3.586558000000	1.500377000000	-2.336678000000
H	-3.084468000000	2.314916000000	-2.865495000000

H	-3.561876000000	0.613528000000	-2.974415000000
H	-4.632158000000	1.787434000000	-2.195023000000
C	-2.892789000000	2.496609000000	-0.132095000000
H	-3.909934000000	2.826993000000	0.095583000000
H	-2.373158000000	2.324269000000	0.813602000000
H	-2.386015000000	3.311360000000	-0.655940000000
C	2.242568000000	1.242233000000	-3.866127000000
H	3.070502000000	1.072069000000	-3.174715000000
H	2.620489000000	1.125609000000	-4.885194000000
H	1.913793000000	2.278930000000	-3.755417000000
C	-0.056719000000	0.532074000000	-4.579726000000
H	0.273550000000	0.315616000000	-5.600019000000
H	-0.916716000000	-0.103982000000	-4.358519000000
H	-0.383792000000	1.575096000000	-4.545064000000
C	2.403384000000	-1.070659000000	1.569385000000
C	1.919237000000	-2.194151000000	2.267782000000
C	3.218337000000	-0.186015000000	2.292641000000
C	2.235730000000	-2.417615000000	3.595455000000
C	3.535667000000	-0.412983000000	3.626497000000
C	3.051695000000	-1.528981000000	4.294355000000
H	1.287731000000	-2.907017000000	1.747239000000
H	3.605240000000	0.692275000000	1.790473000000
H	1.842688000000	-3.298002000000	4.094885000000
H	4.168782000000	0.297704000000	4.149445000000
H	3.300125000000	-1.705975000000	5.334784000000

IPr-III^{Ph}-B

Etot = -1619.498142783356

C	-0.409576000	-0.903960000	0.537216000
C	0.776553000	-1.094528000	-0.139356000
N	-1.439666000	-1.239796000	-0.331529000
C	-1.003689000	-1.639418000	-1.536991000
N	0.356138000	-1.547137000	-1.409250000
H	-0.606763000	-0.654541000	1.564203000
O	1.947036000	-3.228289000	2.219421000
C	2.137037000	-0.938272000	0.278321000
O	3.119632000	-1.508950000	-0.551907000
H	3.240633000	-2.433762000	-0.315047000
C	1.881574000	-2.872721000	3.583645000
H	1.910593000	-3.792792000	4.171142000
H	2.728242000	-2.245600000	3.886930000
H	0.953967000	-2.340458000	3.826742000
H	1.948196000	-2.406577000	1.682527000
C	-2.813359000	-1.164193000	0.039282000
C	-3.509530000	0.032348000	-0.172335000
C	-3.420838000	-2.284238000	0.620334000

C	-4.850266000	0.081726000	0.201020000
C	-4.763484000	-2.186789000	0.977612000
C	-5.474061000	-1.016294000	0.769916000
H	-5.414112000	0.994855000	0.042486000
H	-5.258935000	-3.041546000	1.425741000
C	1.179933000	-1.807438000	-2.548412000
C	1.509516000	-3.130388000	-2.869473000
C	1.580257000	-0.733942000	-3.352581000
C	2.260708000	-3.358575000	-4.019096000
C	2.336162000	-1.009777000	-4.488979000
C	2.676593000	-2.309800000	-4.823040000
H	2.523954000	-4.375496000	-4.290202000
H	2.657412000	-0.192083000	-5.125697000
C	1.063440000	-4.302299000	-2.021468000
H	0.609427000	-3.900169000	-1.113334000
C	1.210797000	0.698266000	-3.032063000
H	0.629988000	0.694340000	-2.107687000
C	-2.853991000	1.246809000	-0.792004000
H	-1.809745000	0.995711000	-0.988512000
C	-2.668386000	-3.574216000	0.862976000
H	-1.643570000	-3.431567000	0.514464000
H	3.262977000	-2.507098000	-5.714161000
H	-6.519427000	-0.959008000	1.054001000
C	-0.001596000	-5.124620000	-2.746604000
H	-0.863398000	-4.507632000	-3.010550000
H	0.401754000	-5.557568000	-3.666678000
H	-0.348378000	-5.945095000	-2.112171000
C	2.230032000	-5.194177000	-1.601980000
H	2.702139000	-5.670112000	-2.465441000
H	2.999044000	-4.630369000	-1.068103000
H	1.874073000	-5.988173000	-0.940164000
C	0.331172000	1.301820000	-4.125955000
H	-0.573998000	0.708945000	-4.278817000
H	0.031708000	2.317797000	-3.854251000
H	0.865906000	1.354218000	-5.078464000
C	2.449413000	1.560320000	-2.794766000
H	2.155233000	2.575747000	-2.515656000
H	3.067308000	1.151013000	-1.992315000
H	3.064059000	1.627332000	-3.696822000
C	-2.608632000	-3.913884000	2.351123000
H	-2.018350000	-4.820681000	2.507826000
H	-2.148334000	-3.105078000	2.923987000
H	-3.608179000	-4.090697000	2.757948000
C	-3.270546000	-4.728748000	0.064300000
H	-3.282744000	-4.505334000	-1.005220000
H	-2.684998000	-5.639479000	0.216042000

H	-4.297212000	-4.934951000	0.379291000
C	-2.871948000	2.440239000	0.161286000
H	-3.894901000	2.757384000	0.382134000
H	-2.380540000	2.198823000	1.107000000
H	-2.348825000	3.288900000	-0.287410000
C	-3.501364000	1.607090000	-2.127966000
H	-3.458401000	0.768354000	-2.826988000
H	-4.550587000	1.886004000	-1.996709000
H	-2.983612000	2.456334000	-2.581927000
C	2.607634000	-0.039801000	1.266874000
C	1.778087000	0.814241000	2.052967000
C	4.006265000	0.069272000	1.534069000
C	2.301663000	1.668647000	3.005909000
C	4.507579000	0.923247000	2.496468000
C	3.670645000	1.738693000	3.259674000
H	0.708513000	0.820405000	1.892848000
H	4.690692000	-0.538863000	0.955867000
H	1.617696000	2.300125000	3.566847000
H	5.582327000	0.956637000	2.654952000
H	4.069466000	2.402467000	4.017862000

IPr-TS1^{iPr}-A $i128\text{ cm}^{-1}$ Etot = -1506.982979887359

H	-1.318603000000	4.084512000000	0.218570000000
C	-2.210053000000	2.182963000000	0.908549000000
C	-1.347737000000	3.009733000000	0.285488000000
N	-1.768150000000	0.899029000000	0.651813000000
C	-0.653056000000	0.887353000000	-0.116661000000
N	-0.408857000000	2.202357000000	-0.329596000000
H	-3.085182000000	2.385870000000	1.503260000000
H	2.588172000000	-1.108585000000	1.527654000000
O	3.139220000000	-1.378084000000	2.296036000000
C	0.614168000000	-0.999088000000	-0.244693000000
O	1.784138000000	-0.721009000000	0.055915000000
C	0.636205000000	2.729357000000	-1.157681000000
C	1.888656000000	2.992383000000	-0.587936000000
C	0.344469000000	3.008977000000	-2.498778000000
C	2.871448000000	3.528002000000	-1.415497000000
C	1.362009000000	3.548340000000	-3.281749000000
C	2.613835000000	3.801123000000	-2.748822000000
H	3.852843000000	3.741242000000	-1.009060000000
H	1.168303000000	3.777296000000	-4.323502000000
C	-2.448275000000	-0.265453000000	1.137792000000
C	-3.394550000000	-0.888345000000	0.313054000000
C	-2.175092000000	-0.709045000000	2.437141000000
C	-4.066801000000	-1.994134000000	0.825845000000
C	-2.878340000000	-1.816854000000	2.903118000000

C	-3.813242000000	-2.455099000000	2.106971000000
H	-4.807008000000	-2.497982000000	0.215334000000
H	-2.690833000000	-2.183070000000	3.906105000000
C	2.161829000000	2.769187000000	0.883999000000
H	1.455560000000	2.016267000000	1.242041000000
C	-1.178926000000	-0.014149000000	3.339685000000
H	-0.616689000000	0.701645000000	2.735491000000
C	-3.737940000000	-0.360891000000	-1.063456000000
H	-2.918687000000	0.284414000000	-1.388890000000
C	-1.032431000000	2.796920000000	-3.092405000000
H	-1.608600000000	2.180748000000	-2.398598000000
H	-0.074659000000	-1.359837000000	0.535898000000
C	4.360166000000	-1.874983000000	1.799313000000
H	4.925706000000	-1.110980000000	1.250418000000
H	4.967096000000	-2.199595000000	2.647380000000
H	4.216801000000	-2.736746000000	1.135227000000
H	3.394254000000	4.219516000000	-3.375164000000
H	-4.350599000000	-3.316833000000	2.487751000000
C	3.567115000000	2.246715000000	1.162174000000
H	3.659673000000	1.990391000000	2.220282000000
H	3.784895000000	1.351642000000	0.576553000000
H	4.329879000000	2.997525000000	0.941006000000
C	1.913333000000	4.059237000000	1.669321000000
H	0.894952000000	4.428277000000	1.530702000000
H	2.071436000000	3.888512000000	2.737499000000
H	2.604363000000	4.842706000000	1.344863000000
C	-1.900692000000	0.768715000000	4.436980000000
H	-2.593013000000	1.501915000000	4.016625000000
H	-2.471842000000	0.094290000000	5.081202000000
H	-1.177329000000	1.299998000000	5.060970000000
C	-0.172810000000	-0.988724000000	3.945708000000
H	-0.657222000000	-1.697322000000	4.622208000000
H	0.348017000000	-1.557126000000	3.172264000000
H	0.574728000000	-0.439221000000	4.523230000000
C	-5.006826000000	0.491873000000	-1.002389000000
H	-5.230100000000	0.910711000000	-1.987218000000
H	-5.861749000000	-0.114601000000	-0.689717000000
H	-4.901882000000	1.318344000000	-0.295960000000
C	-3.888216000000	-1.465770000000	-2.104776000000
H	-3.004843000000	-2.107328000000	-2.140863000000
H	-4.757630000000	-2.096496000000	-1.903663000000
H	-4.028005000000	-1.022715000000	-3.093883000000
C	-0.996196000000	2.062462000000	-4.429849000000
H	-0.493411000000	2.652174000000	-5.200297000000
H	-0.482898000000	1.102653000000	-4.347087000000
H	-2.016299000000	1.874574000000	-4.774223000000

C	-1.758041000000	4.135621000000	-3.240178000000
H	-1.227158000000	4.785348000000	-3.941808000000
H	-2.769390000000	3.977999000000	-3.624046000000
H	-1.832949000000	4.659954000000	-2.284913000000
C	0.252361000000	-1.476005000000	-1.635671000000
H	-0.794735000000	-1.218813000000	-1.810936000000
C	0.374567000000	-3.002435000000	-1.631514000000
H	0.055980000000	-3.407726000000	-2.595060000000
H	1.409847000000	-3.310745000000	-1.460623000000
H	-0.248717000000	-3.453340000000	-0.854416000000
C	1.123414000000	-0.855535000000	-2.710487000000
H	2.171362000000	-1.126801000000	-2.562595000000
H	0.819422000000	-1.206227000000	-3.699817000000
H	1.054309000000	0.234024000000	-2.694699000000

IPr-II^{iPr}-A

Etot = -1507.011145701613

C	-0.367164000000	-0.351425000000	0.018043000000
C	-1.162642000000	-2.070756000000	-1.162140000000
H	-1.911002000000	-2.665017000000	-1.657228000000
C	0.161700000000	-2.257921000000	-1.007667000000
H	0.810441000000	-3.048507000000	-1.344081000000
N	-1.474816000000	-0.887544000000	-0.527461000000
N	0.643039000000	-1.191366000000	-0.279686000000
C	2.037496000000	-1.089034000000	0.072586000000
C	2.913803000000	-0.496389000000	-0.844907000000
C	2.471671000000	-1.683874000000	1.263060000000
C	4.262595000000	-0.450111000000	-0.502671000000
C	3.830863000000	-1.609055000000	1.553393000000
C	4.716212000000	-0.989121000000	0.688411000000
H	4.969053000000	0.005745000000	-1.186287000000
H	4.202623000000	-2.055604000000	2.468201000000
C	-2.815922000000	-0.364586000000	-0.481569000000
C	-3.601234000000	-0.641787000000	0.645164000000
C	-3.302339000000	0.326201000000	-1.597910000000
C	-4.906218000000	-0.159685000000	0.646493000000
C	-4.617038000000	0.782373000000	-1.542099000000
C	-5.408237000000	0.550154000000	-0.431419000000
H	-5.542685000000	-0.349957000000	1.502184000000
H	-5.027537000000	1.323079000000	-2.386773000000
C	-2.489459000000	0.534328000000	-2.857976000000
H	-1.441734000000	0.325035000000	-2.628823000000
C	-3.096689000000	-1.488006000000	1.794009000000
H	-2.005094000000	-1.437746000000	1.798477000000
C	2.464024000000	0.017251000000	-2.195993000000
H	1.376559000000	0.119277000000	-2.179764000000

C	1.546370000000	-2.457939000000	2.174426000000
H	0.522355000000	-2.193319000000	1.909374000000
C	-0.346823000000	0.831767000000	0.980164000000
O	-0.031094000000	0.332199000000	2.199299000000
H	-0.332044000000	0.984023000000	3.573483000000
O	-0.446140000000	1.251473000000	4.546857000000
C	-1.365519000000	2.303043000000	4.651659000000
H	-1.632041000000	2.438568000000	5.704398000000
H	-0.959171000000	3.257155000000	4.286296000000
H	-2.294855000000	2.106992000000	4.098949000000
H	-1.384278000000	1.231538000000	0.920351000000
H	-6.428640000000	0.916751000000	-0.408660000000
H	5.770996000000	-0.941442000000	0.936291000000
C	-3.568747000000	-0.989035000000	3.155359000000
H	-3.070476000000	-1.555876000000	3.945341000000
H	-3.335696000000	0.068151000000	3.297130000000
H	-4.645327000000	-1.122461000000	3.286863000000
C	-3.509856000000	-2.947551000000	1.590667000000
H	-3.132075000000	-3.349488000000	0.648012000000
H	-3.122783000000	-3.566385000000	2.404373000000
H	-4.599849000000	-3.038589000000	1.584424000000
C	-2.933577000000	-0.447313000000	-3.944897000000
H	-2.845069000000	-1.485338000000	-3.617937000000
H	-3.976984000000	-0.267751000000	-4.218475000000
H	-2.321381000000	-0.318103000000	-4.841084000000
C	-2.567881000000	1.965497000000	-3.383297000000
H	-3.568261000000	2.201383000000	-3.754045000000
H	-2.309310000000	2.693690000000	-2.613100000000
H	-1.871685000000	2.088518000000	-4.216595000000
C	2.814682000000	-0.995467000000	-3.288770000000
H	3.898050000000	-1.129843000000	-3.352471000000
H	2.364112000000	-1.971602000000	-3.096840000000
H	2.459266000000	-0.640085000000	-4.259412000000
C	3.049069000000	1.384248000000	-2.538920000000
H	2.857101000000	2.114937000000	-1.751045000000
H	4.128845000000	1.329491000000	-2.696968000000
H	2.600351000000	1.754083000000	-3.464115000000
C	1.726611000000	-2.095003000000	3.644059000000
H	0.993763000000	-2.636384000000	4.248206000000
H	2.719117000000	-2.364266000000	4.014005000000
H	1.568605000000	-1.026143000000	3.790578000000
C	1.734289000000	-3.960965000000	1.958245000000
H	2.745399000000	-4.270323000000	2.238250000000
H	1.026668000000	-4.521214000000	2.575186000000
H	1.573338000000	-4.242843000000	0.914834000000
C	0.552706000000	1.990187000000	0.485997000000

H	1.561769000000	1.591068000000	0.331850000000
C	0.042766000000	2.593549000000	-0.812207000000
H	0.690545000000	3.408267000000	-1.145156000000
H	-0.009087000000	1.863633000000	-1.623304000000
H	-0.960958000000	3.006406000000	-0.669643000000
C	0.629064000000	3.060924000000	1.562669000000
H	-0.361599000000	3.490711000000	1.747668000000
H	0.999611000000	2.653426000000	2.503433000000
H	1.291069000000	3.872608000000	1.248660000000

IPr-TS2^{iPr}-A $i1316\text{ cm}^{-1}$ Etot = -1506.971313765101

C	-0.361649000000	-0.070380000000	0.020819000000
C	-1.168471000000	-2.073801000000	-0.604178000000
H	-1.929138000000	-2.806571000000	-0.810291000000
C	0.167604000000	-2.149292000000	-0.658811000000
H	0.822189000000	-2.956597000000	-0.937731000000
N	-1.496564000000	-0.794446000000	-0.187782000000
N	0.666939000000	-0.916340000000	-0.279589000000
C	2.082467000000	-0.668076000000	-0.307774000000
C	2.860959000000	-1.109391000000	0.770612000000
C	2.643401000000	-0.099999000000	-1.459805000000
C	4.238866000000	-0.930284000000	0.686904000000
C	4.025324000000	0.065965000000	-1.484846000000
C	4.815983000000	-0.340315000000	-0.423419000000
H	4.868430000000	-1.260809000000	1.504848000000
H	4.492418000000	0.507249000000	-2.356752000000
C	-2.882416000000	-0.459436000000	0.018007000000
C	-3.463061000000	-0.755848000000	1.255109000000
C	-3.627066000000	0.014576000000	-1.069310000000
C	-4.829679000000	-0.529362000000	1.397912000000
C	-4.988537000000	0.224176000000	-0.872561000000
C	-5.586514000000	-0.040222000000	0.348373000000
H	-5.308185000000	-0.747066000000	2.346044000000
H	-5.593055000000	0.595489000000	-1.691478000000
C	-3.010375000000	0.258408000000	-2.430351000000
H	-1.935110000000	0.398180000000	-2.293259000000
C	-2.679531000000	-1.340946000000	2.409939000000
H	-1.616182000000	-1.278148000000	2.168034000000
C	2.266666000000	-1.793402000000	1.983082000000
H	1.186401000000	-1.628923000000	1.969931000000
C	1.812180000000	0.248493000000	-2.675544000000
H	0.790338000000	0.446171000000	-2.343928000000
C	-0.263790000000	1.338987000000	0.353894000000
O	-1.544219000000	1.883446000000	0.645575000000
H	-1.713042000000	2.459595000000	-0.119818000000

H	-0.107176000000	2.048977000000	-0.786409000000
O	-0.550697000000	2.804690000000	-1.707306000000
C	-0.023154000000	4.084027000000	-1.793933000000
H	-0.355843000000	4.751979000000	-0.980191000000
H	1.080549000000	4.102542000000	-1.777805000000
H	-0.324690000000	4.567277000000	-2.737076000000
C	-3.023944000000	-2.819040000000	2.599971000000
H	-2.428506000000	-3.245559000000	3.411502000000
H	-4.080167000000	-2.938896000000	2.856993000000
H	-2.829036000000	-3.396602000000	1.693437000000
C	-2.900181000000	-0.570294000000	3.709153000000
H	-2.245841000000	-0.964950000000	4.490554000000
H	-2.681327000000	0.492134000000	3.586459000000
H	-3.929965000000	-0.667884000000	4.061707000000
C	-3.545547000000	1.517288000000	-3.106109000000
H	-4.594216000000	1.407508000000	-3.393585000000
H	-3.454951000000	2.389345000000	-2.456076000000
H	-2.975638000000	1.713906000000	-4.017339000000
C	-3.220879000000	-0.951507000000	-3.343677000000
H	-4.288271000000	-1.118657000000	-3.514736000000
H	-2.745653000000	-0.779263000000	-4.313121000000
H	-2.800693000000	-1.864525000000	-2.917804000000
C	2.298656000000	1.500747000000	-3.395772000000
H	2.381532000000	2.349520000000	-2.714589000000
H	3.269445000000	1.343545000000	-3.872489000000
H	1.588869000000	1.767589000000	-4.182098000000
C	2.509902000000	-3.302731000000	1.923647000000
H	2.047929000000	-3.792464000000	2.784764000000
H	2.094907000000	-3.746584000000	1.016473000000
H	3.581663000000	-3.519120000000	1.946009000000
C	2.803922000000	-1.226785000000	3.294936000000
H	2.683950000000	-0.143228000000	3.344709000000
H	2.263858000000	-1.668603000000	4.135909000000
H	3.863464000000	-1.458932000000	3.426764000000
H	-6.649823000000	0.129014000000	0.478804000000
H	5.891179000000	-0.205373000000	-0.467616000000
C	1.777836000000	-0.934371000000	-3.646834000000
H	2.783299000000	-1.151678000000	-4.018714000000
H	1.388908000000	-1.839179000000	-3.175725000000
H	1.142482000000	-0.698097000000	-4.504529000000
C	0.751018000000	1.722526000000	1.433728000000
H	1.663320000000	1.148521000000	1.255642000000
C	0.249819000000	1.391724000000	2.837703000000
H	-0.658611000000	1.954611000000	3.063476000000
H	0.023983000000	0.328554000000	2.948968000000
H	1.001865000000	1.656554000000	3.586117000000

C	1.121377000000	3.198068000000	1.351188000000
H	1.808522000000	3.463995000000	2.159147000000
H	1.601501000000	3.439068000000	0.401187000000
H	0.232347000000	3.827225000000	1.448965000000

IPr-III^{iPr}-A

Etot = -1506.991808116759

C	-0.253468000000	-0.273069000000	-0.021220000000
C	-1.134837000000	-2.172832000000	-0.928250000000
H	-1.915019000000	-2.854659000000	-1.221810000000
C	0.183974000000	-2.224642000000	-1.123865000000
H	0.795526000000	-2.978506000000	-1.589794000000
N	-1.432844000000	-0.992252000000	-0.247058000000
N	0.756508000000	-1.071033000000	-0.579864000000
C	2.143166000000	-1.043982000000	-0.247488000000
C	3.050403000000	-0.502781000000	-1.171179000000
C	2.573027000000	-1.622053000000	0.956593000000
C	4.405684000000	-0.535213000000	-0.856871000000
C	3.938400000000	-1.620819000000	1.231552000000
C	4.847315000000	-1.081791000000	0.336990000000
H	5.127111000000	-0.127398000000	-1.555841000000
H	4.296711000000	-2.065247000000	2.153737000000
C	-2.776724000000	-0.531442000000	-0.129894000000
C	-3.556385000000	-0.989863000000	0.941412000000
C	-3.310494000000	0.298422000000	-1.125985000000
C	-4.887598000000	-0.588413000000	1.004499000000
C	-4.644332000000	0.682936000000	-1.014305000000
C	-5.428339000000	0.245821000000	0.040171000000
H	-5.510787000000	-0.933627000000	1.822294000000
H	-5.079816000000	1.323715000000	-1.773322000000
C	-2.500670000000	0.737407000000	-2.327021000000
H	-1.457955000000	0.469290000000	-2.145407000000
C	-2.995183000000	-1.913484000000	1.999987000000
H	-1.912970000000	-1.954988000000	1.856890000000
C	2.583815000000	0.074975000000	-2.489460000000
H	1.508759000000	0.252241000000	-2.402136000000
C	1.615912000000	-2.303215000000	1.911605000000
H	0.598231000000	-2.067773000000	1.594245000000
C	-0.130724000000	0.931455000000	0.599730000000
O	-1.265737000000	1.423597000000	1.264210000000
H	-1.409157000000	1.774532000000	3.055912000000
O	-1.538142000000	1.988385000000	3.997816000000
C	-2.435142000000	3.074634000000	4.079426000000
H	-2.569111000000	3.321416000000	5.134180000000
H	-2.051153000000	3.964878000000	3.566623000000
H	-3.417847000000	2.830154000000	3.658019000000

H	-1.724713000000	2.068064000000	0.712868000000
H	-6.467049000000	0.551297000000	0.106958000000
H	5.907288000000	-1.095640000000	0.567069000000
C	1.784537000000	-3.821844000000	1.836268000000
H	1.057145000000	-4.316137000000	2.485855000000
H	1.638232000000	-4.189475000000	0.818063000000
H	2.785516000000	-4.117059000000	2.163684000000
C	1.768607000000	-1.823050000000	3.351998000000
H	1.620603000000	-0.744398000000	3.432602000000
H	1.026747000000	-2.314682000000	3.986661000000
H	2.756531000000	-2.061994000000	3.754054000000
C	-3.255648000000	-1.403415000000	3.415010000000
H	-4.323832000000	-1.390717000000	3.647282000000
H	-2.769352000000	-2.059557000000	4.141795000000
H	-2.865037000000	-0.392995000000	3.554380000000
C	-3.542464000000	-3.331008000000	1.830864000000
H	-3.322129000000	-3.729926000000	0.837874000000
H	-3.100452000000	-4.000804000000	2.573467000000
H	-4.627796000000	-3.345630000000	1.967215000000
C	-2.958323000000	-0.006194000000	-3.582507000000
H	-2.881717000000	-1.088511000000	-3.453954000000
H	-3.999015000000	0.234380000000	-3.818129000000
H	-2.343204000000	0.280387000000	-4.439788000000
C	-2.553997000000	2.246889000000	-2.548018000000
H	-1.898228000000	2.526353000000	-3.376657000000
H	-3.563864000000	2.580587000000	-2.799881000000
H	-2.228677000000	2.793853000000	-1.659948000000
C	2.798652000000	-0.930144000000	-3.622037000000
H	2.423500000000	-0.526035000000	-4.566160000000
H	3.863712000000	-1.147018000000	-3.746005000000
H	2.282879000000	-1.872779000000	-3.425414000000
C	3.250350000000	1.406221000000	-2.824371000000
H	3.127237000000	2.131535000000	-2.016823000000
H	4.320329000000	1.287301000000	-3.013062000000
H	2.803305000000	1.826053000000	-3.729036000000
C	1.053696000000	1.850775000000	0.592723000000
H	1.858132000000	1.351779000000	0.051060000000
C	1.571792000000	2.176070000000	1.993991000000
H	0.793215000000	2.650158000000	2.597080000000
H	1.898497000000	1.273225000000	2.513916000000
H	2.419494000000	2.865518000000	1.942565000000
C	0.740754000000	3.150171000000	-0.158541000000
H	1.618257000000	3.802692000000	-0.181528000000
H	0.436501000000	2.948870000000	-1.188576000000
H	-0.064460000000	3.706120000000	0.331831000000

IPr-TS1^{iPr}-B $i208\text{ cm}^{-1}$ Etot = -1506.462981512803

C	-0.301571000000	-0.729291000000	0.209484000000
C	0.761978000000	-1.101250000000	-0.547029000000
N	-1.462525000000	-1.041247000000	-0.495916000000
C	-1.194432000000	-1.601670000000	-1.697449000000
N	0.170604000000	-1.621826000000	-1.699153000000
H	-0.351560000000	-0.278364000000	1.187907000000
O	5.353840000000	1.678674000000	-0.885268000000
C	2.835813000000	-0.914756000000	-0.366673000000
O	3.256085000000	0.110197000000	-1.005728000000
C	6.393226000000	1.019755000000	-1.563998000000
H	6.099773000000	0.712371000000	-2.576444000000
H	7.239979000000	1.705013000000	-1.654638000000
H	6.741112000000	0.126168000000	-1.027599000000
H	4.566412000000	1.073452000000	-0.872241000000
C	-2.777074000000	-0.780447000000	-0.011203000000
C	-3.366651000000	0.461376000000	-0.283723000000
C	-3.434253000000	-1.760472000000	0.744008000000
C	-4.644912000000	0.702416000000	0.213122000000
C	-4.712429000000	-1.474324000000	1.217114000000
C	-5.315151000000	-0.255245000000	0.955936000000
H	-5.122172000000	1.656185000000	0.014702000000
H	-5.243035000000	-2.219587000000	1.800093000000
C	0.909677000000	-2.163959000000	-2.794095000000
C	1.363213000000	-3.488267000000	-2.718365000000
C	1.149814000000	-1.368289000000	-3.922599000000
C	2.069619000000	-4.004560000000	-3.801501000000
C	1.858745000000	-1.929830000000	-4.982452000000
C	2.318263000000	-3.234455000000	-4.925393000000
H	2.423908000000	-5.029190000000	-3.767025000000
H	2.050812000000	-1.334493000000	-5.868663000000
C	1.065613000000	-4.374571000000	-1.527709000000
H	0.639326000000	-3.745252000000	-0.743986000000
C	0.639105000000	0.052097000000	-4.037327000000
H	0.217922000000	0.331834000000	-3.069652000000
C	-2.659553000000	1.530396000000	-1.087921000000
H	-1.698764000000	1.123583000000	-1.409455000000
C	-2.803234000000	-3.100364000000	1.052918000000
H	-1.809379000000	-3.111793000000	0.601104000000
H	2.868893000000	-3.653850000000	-5.760710000000
H	-6.310952000000	-0.049993000000	1.334034000000
C	0.024284000000	-5.432718000000	-1.893146000000
H	-0.900098000000	-4.972590000000	-2.250502000000
H	0.400684000000	-6.093058000000	-2.679850000000
H	-0.214214000000	-6.049009000000	-1.021907000000

C	2.321199000000	-5.030908000000	-0.959026000000
H	2.773544000000	-5.722574000000	-1.674677000000
H	3.072478000000	-4.285451000000	-0.687383000000
H	2.070033000000	-5.602815000000	-0.061798000000
C	-0.480750000000	0.141933000000	-5.074210000000
H	-1.299145000000	-0.540455000000	-4.833655000000
H	-0.881997000000	1.158409000000	-5.113987000000
H	-0.108678000000	-0.111932000000	-6.071111000000
C	1.752365000000	1.045019000000	-4.364289000000
H	1.349383000000	2.061122000000	-4.390616000000
H	2.545393000000	1.012514000000	-3.614092000000
H	2.197482000000	0.841507000000	-5.341925000000
C	-2.630840000000	-3.303140000000	2.557137000000
H	-2.126731000000	-4.252955000000	2.754499000000
H	-2.033190000000	-2.502168000000	2.999203000000
H	-3.597337000000	-3.325496000000	3.068099000000
C	-3.604690000000	-4.246011000000	0.437412000000
H	-3.691918000000	-4.130484000000	-0.645645000000
H	-3.116326000000	-5.202695000000	0.640909000000
H	-4.614088000000	-4.290622000000	0.855719000000
C	-2.379612000000	2.768694000000	-0.237970000000
H	-3.310301000000	3.229886000000	0.104274000000
H	-1.782369000000	2.518710000000	0.642317000000
H	-1.831531000000	3.513054000000	-0.821729000000
C	-3.445721000000	1.898920000000	-2.344611000000
H	-3.633305000000	1.019749000000	-2.965723000000
H	-4.410536000000	2.347955000000	-2.093511000000
H	-2.885518000000	2.624567000000	-2.940336000000
C	3.025605000000	-0.993778000000	1.144644000000
H	2.381408000000	-1.800473000000	1.509387000000
C	4.476165000000	-1.382522000000	1.432138000000
H	4.645006000000	-1.483899000000	2.508075000000
H	4.734440000000	-2.335222000000	0.960668000000
H	5.163164000000	-0.619432000000	1.055236000000
C	2.665858000000	0.299693000000	1.859180000000
H	3.418258000000	1.067005000000	1.661789000000
H	1.698294000000	0.685471000000	1.532941000000
H	2.626690000000	0.145678000000	2.940978000000
H	3.004639000000	-1.903369000000	-0.830484000000

IPr-II^{iPr}-B

Etot = -1506.508787655964

C	-0.689608000000	-0.592241000000	0.645155000000
C	0.504731000000	-0.989591000000	0.147784000000
N	-1.663483000000	-1.000879000000	-0.248948000000
C	-1.147414000000	-1.655151000000	-1.316128000000

N	0.18824000000	-1.63034100000	-1.05188100000
H	-0.93214100000	-0.06466500000	1.55282300000
O	1.31249300000	2.48665100000	-0.18898200000
C	1.91551800000	-0.75956000000	0.64594200000
O	2.50219900000	0.29883200000	-0.00056200000
H	1.77677900000	1.55020900000	-0.08094700000
C	2.19098200000	3.47639500000	0.25828000000
H	2.53014800000	3.30542200000	1.29187900000
H	3.09234400000	3.56094100000	-0.36916100000
H	1.68999800000	4.45068000000	0.23813000000
H	2.46826300000	-1.70183200000	0.43090600000
C	-3.05693900000	-0.76405300000	-0.05186700000
C	-3.61746900000	0.42422900000	-0.53690300000
C	-3.81620000000	-1.71726000000	0.63826800000
C	-4.97553500000	0.64057600000	-0.31815200000
C	-5.17065900000	-1.45667500000	0.82984400000
C	-5.74731100000	-0.28933400000	0.35816600000
H	-5.43465400000	1.55288600000	-0.68343700000
H	-5.78187400000	-2.17995800000	1.35896100000
C	1.13312700000	-2.23546500000	-1.93895500000
C	1.53588500000	-1.53860600000	-3.08687900000
C	1.59485300000	-3.52884100000	-1.65914700000
C	2.41947200000	-2.17166400000	-3.95761300000
C	2.48181800000	-4.11634700000	-2.55773300000
C	2.89236600000	-3.44654200000	-3.69759600000
H	2.73946800000	-1.65744000000	-4.85705000000
H	2.84758500000	-5.11911400000	-2.36714300000
C	1.01572400000	-0.15791500000	-3.42543300000
H	0.50744600000	0.23132000000	-2.54104800000
C	1.11211200000	-4.31610800000	-0.45970100000
H	0.60379900000	-3.62370400000	0.21434000000
C	-2.79976800000	1.46274600000	-1.27303200000
H	-1.78482800000	1.07519300000	-1.38021000000
C	-3.21543100000	-2.99849600000	1.17403700000
H	-2.15576900000	-3.00654900000	0.91152100000
H	3.58047600000	-3.92186600000	-4.38848200000
H	-6.80378500000	-0.10313700000	0.51880100000
C	2.13481900000	0.81799400000	-3.78134700000
H	2.88124600000	0.87479700000	-2.98627300000
H	2.64218100000	0.53119000000	-4.70608700000
H	1.72000200000	1.81829100000	-3.93088900000
C	-0.00892100000	-0.23046200000	-4.55773300000
H	0.45107400000	-0.61632400000	-5.47227700000
H	-0.84349000000	-0.88285700000	-4.29262500000
H	-0.40635000000	0.76500300000	-4.77462400000
C	-3.34477200000	1.71391800000	-2.67743600000

H	-3.379202000000	0.790086000000	-3.259884000000
H	-4.354838000000	2.131068000000	-2.643664000000
H	-2.706780000000	2.426980000000	-3.206163000000
C	-2.716887000000	2.765499000000	-0.478946000000
H	-3.706550000000	3.213476000000	-0.352802000000
H	-2.291309000000	2.598793000000	0.513530000000
H	-2.084962000000	3.487570000000	-1.002696000000
C	-3.857001000000	-4.226491000000	0.530817000000
H	-3.760193000000	-4.199332000000	-0.557208000000
H	-3.374556000000	-5.137947000000	0.893693000000
H	-4.920857000000	-4.291097000000	0.775067000000
C	-3.315640000000	-3.065529000000	2.696985000000
H	-4.358816000000	-3.083447000000	3.024412000000
H	-2.833006000000	-3.973955000000	3.067071000000
H	-2.828959000000	-2.206246000000	3.164827000000
C	0.092716000000	-5.371087000000	-0.891870000000
H	-0.291587000000	-5.909125000000	-0.020900000000
H	-0.752153000000	-4.915102000000	-1.413243000000
H	0.553021000000	-6.100844000000	-1.564339000000
C	2.254680000000	-4.959903000000	0.320580000000
H	2.996441000000	-4.217984000000	0.625315000000
H	1.865161000000	-5.440605000000	1.221686000000
H	2.763500000000	-5.728075000000	-0.267357000000
C	1.930369000000	-0.635498000000	2.190096000000
H	1.268847000000	0.199920000000	2.459074000000
C	1.440944000000	-1.897649000000	2.890215000000
H	1.463411000000	-1.772939000000	3.976805000000
H	0.422023000000	-2.164035000000	2.603477000000
H	2.089838000000	-2.745096000000	2.644222000000
C	3.332728000000	-0.296543000000	2.672723000000
H	3.350919000000	-0.170425000000	3.759197000000
H	4.029217000000	-1.104735000000	2.420533000000
H	3.700365000000	0.618984000000	2.209391000000

IPr-TS2^{iPr}-B ν 115 cm⁻¹ Etot = -1506.453144965230

C	-0.280061000000	-0.908647000000	0.399879000000
C	0.860737000000	-1.082665000000	-0.335624000000
N	-1.357072000000	-1.267293000000	-0.400015000000
C	-0.979874000000	-1.644098000000	-1.638715000000
N	0.379415000000	-1.534041000000	-1.582418000000
H	-0.418380000000	-0.563321000000	1.409854000000
O	4.373421000000	-2.499470000000	-0.425504000000
C	2.259986000000	-0.880779000000	0.030010000000
O	2.842670000000	0.017398000000	-0.956688000000
H	3.717733000000	-0.325866000000	-1.154249000000

C	4.838632000000	-3.275581000000	0.639216000000
H	5.311201000000	-2.673230000000	1.431051000000
H	4.037511000000	-3.859736000000	1.116397000000
H	5.591418000000	-3.984817000000	0.276573000000
H	3.450798000000	-2.030661000000	-0.152475000000
C	-2.709359000000	-1.222706000000	0.046872000000
C	-3.472006000000	-0.075473000000	-0.208665000000
C	-3.234313000000	-2.318753000000	0.745342000000
C	-4.790027000000	-0.051853000000	0.241007000000
C	-4.554687000000	-2.245211000000	1.181329000000
C	-5.329016000000	-1.124552000000	0.930572000000
H	-5.401645000000	0.823728000000	0.050797000000
H	-4.983939000000	-3.081279000000	1.723033000000
C	1.178845000000	-1.938360000000	-2.696903000000
C	1.502172000000	-1.007604000000	-3.693396000000
C	1.566091000000	-3.283537000000	-2.793699000000
C	2.245908000000	-1.446893000000	-4.785501000000
C	2.315672000000	-3.673363000000	-3.901295000000
C	2.657480000000	-2.764994000000	-4.888416000000
H	2.503547000000	-0.745585000000	-5.571536000000
H	2.626777000000	-4.707282000000	-3.998205000000
C	1.021114000000	0.425362000000	-3.642742000000
H	0.657194000000	0.612257000000	-2.631245000000
C	1.130466000000	-4.317512000000	-1.776388000000
H	0.859775000000	-3.784622000000	-0.861494000000
C	-2.909313000000	1.122139000000	-0.941994000000
H	-1.870939000000	0.898586000000	-1.194097000000
C	-2.415458000000	-3.557133000000	1.036751000000
H	-1.454799000000	-3.446022000000	0.529665000000
H	3.239664000000	-3.087174000000	-5.745371000000
H	-6.356924000000	-1.087151000000	1.275195000000
C	-0.114737000000	-5.051677000000	-2.276594000000
H	0.108601000000	-5.599634000000	-3.197115000000
H	-0.459224000000	-5.772073000000	-1.529428000000
H	-0.926585000000	-4.350719000000	-2.480312000000
C	2.223489000000	-5.319143000000	-1.418864000000
H	3.129998000000	-4.812876000000	-1.083560000000
H	1.875524000000	-5.969571000000	-0.611946000000
H	2.478719000000	-5.961704000000	-2.265650000000
C	-3.081853000000	-4.818252000000	0.491316000000
H	-3.267423000000	-4.736407000000	-0.582268000000
H	-2.438578000000	-5.685874000000	0.659914000000
H	-4.037060000000	-5.011631000000	0.986728000000
C	-2.138965000000	-3.693918000000	2.533465000000
H	-3.069579000000	-3.820414000000	3.094077000000
H	-1.510084000000	-4.567556000000	2.724910000000

H	-1.625476000000	-2.812066000000	2.924233000000
C	-3.656105000000	1.378025000000	-2.249642000000
H	-3.201111000000	2.214047000000	-2.787620000000
H	-3.628610000000	0.499673000000	-2.898986000000
H	-4.704024000000	1.630188000000	-2.064582000000
C	-2.915579000000	2.368564000000	-0.058572000000
H	-3.934538000000	2.655591000000	0.215531000000
H	-2.351110000000	2.203845000000	0.862501000000
H	-2.462742000000	3.209918000000	-0.589913000000
C	2.131996000000	1.431994000000	-3.925430000000
H	2.969322000000	1.289256000000	-3.240687000000
H	2.502482000000	1.350064000000	-4.950764000000
H	1.752985000000	2.449631000000	-3.796193000000
C	-0.143908000000	0.631330000000	-4.612002000000
H	0.177500000000	0.464554000000	-5.644515000000
H	-0.965600000000	-0.055671000000	-4.397574000000
H	-0.524566000000	1.654174000000	-4.539074000000
C	2.386505000000	-0.288893000000	1.432967000000
H	1.640217000000	0.519990000000	1.577982000000
C	2.138105000000	-1.347672000000	2.506549000000
H	2.049878000000	-0.892042000000	3.498680000000
H	1.229163000000	-1.922338000000	2.319006000000
H	2.978829000000	-2.048470000000	2.532097000000
C	3.753736000000	0.340818000000	1.673727000000
H	3.816802000000	0.739800000000	2.690992000000
H	4.548397000000	-0.402698000000	1.554609000000
H	3.950433000000	1.155902000000	0.975919000000

IPr-III^{iPr}-B

Etot = -1506.445443929113

C	-0.325074000000	-0.785720000000	0.309528000000
C	0.793091000000	-1.106425000000	-0.445284000000
N	-1.450208000000	-1.078372000000	-0.464512000000
C	-1.144693000000	-1.517541000000	-1.693937000000
N	0.226062000000	-1.533780000000	-1.673943000000
H	-0.420385000000	-0.382434000000	1.301489000000
O	4.883291000000	1.249903000000	-1.367140000000
C	2.176771000000	-1.164986000000	-0.131095000000
O	3.028757000000	-0.749792000000	-1.236388000000
H	3.447870000000	-1.535426000000	-1.591580000000
C	6.061317000000	0.642855000000	-1.845906000000
H	5.913454000000	0.165361000000	-2.823052000000
H	6.822056000000	1.417959000000	-1.960406000000
H	6.449477000000	-0.113040000000	-1.151476000000
H	4.201133000000	0.550622000000	-1.264931000000
C	-2.777349000000	-0.875655000000	0.005251000000

C	-3.418539000000	0.340031000000	-0.268145000000
C	-3.401506000000	-1.887931000000	0.746068000000
C	-4.718799000000	0.515607000000	0.200359000000
C	-4.701143000000	-1.666755000000	1.194831000000
C	-5.357553000000	-0.477312000000	0.923831000000
H	-5.237583000000	1.446181000000	-0.004546000000
H	-5.207988000000	-2.440545000000	1.761683000000
C	0.947636000000	-2.034064000000	-2.797769000000
C	1.362686000000	-3.373453000000	-2.800365000000
C	1.178571000000	-1.198377000000	-3.899852000000
C	2.025710000000	-3.857776000000	-3.925788000000
C	1.837063000000	-1.728597000000	-5.005953000000
C	2.263762000000	-3.045920000000	-5.021890000000
H	2.347658000000	-4.893348000000	-3.949179000000
H	2.018831000000	-1.098088000000	-5.869984000000
C	1.056563000000	-4.310838000000	-1.652332000000
H	0.705927000000	-3.700458000000	-0.818554000000
C	0.726594000000	0.245444000000	-3.926193000000
H	0.324387000000	0.480853000000	-2.938841000000
C	-2.743965000000	1.449042000000	-1.045175000000
H	-1.739464000000	1.106283000000	-1.301563000000
C	-2.713683000000	-3.200816000000	1.048930000000
H	-1.703304000000	-3.144661000000	0.639133000000
H	2.777165000000	-3.441867000000	-5.891734000000
H	-6.370767000000	-0.323237000000	1.279606000000
C	-0.061196000000	-5.280988000000	-2.036084000000
H	-0.963094000000	-4.745922000000	-2.342975000000
H	0.248983000000	-5.923997000000	-2.865177000000
H	-0.316763000000	-5.923693000000	-1.188758000000
C	2.287685000000	-5.075702000000	-1.174619000000
H	2.675143000000	-5.745021000000	-1.947268000000
H	3.087697000000	-4.390977000000	-0.882318000000
H	2.033155000000	-5.689189000000	-0.306197000000
C	-0.392185000000	0.452612000000	-4.946478000000
H	-1.245488000000	-0.196208000000	-4.735824000000
H	-0.738550000000	1.489851000000	-4.927331000000
H	-0.041051000000	0.234897000000	-5.959526000000
C	1.883809000000	1.203854000000	-4.199166000000
H	1.533752000000	2.238675000000	-4.149420000000
H	2.682407000000	1.077614000000	-3.465297000000
H	2.307246000000	1.046287000000	-5.194835000000
C	-2.592068000000	-3.438243000000	2.552785000000
H	-2.043502000000	-4.364271000000	2.745018000000
H	-2.059518000000	-2.618764000000	3.042020000000
H	-3.575773000000	-3.530515000000	3.021647000000
C	-3.427626000000	-4.369182000000	0.370826000000

H	-3.483282000000	-4.224304000000	-0.710785000000
H	-2.893024000000	-5.303530000000	0.562644000000
H	-4.446905000000	-4.482473000000	0.750588000000
C	-2.604912000000	2.715945000000	-0.202669000000
H	-3.583127000000	3.120096000000	0.072079000000
H	-2.049276000000	2.519756000000	0.717558000000
H	-2.071346000000	3.487144000000	-0.764668000000
C	-3.480254000000	1.744172000000	-2.350768000000
H	-3.553224000000	0.849706000000	-2.974122000000
H	-4.493982000000	2.107758000000	-2.160059000000
H	-2.950921000000	2.513816000000	-2.918967000000
C	2.689174000000	-0.574141000000	1.163721000000
H	3.779329000000	-0.703901000000	1.118068000000
C	2.442390000000	0.933984000000	1.336705000000
H	2.938806000000	1.322592000000	2.233120000000
H	2.823836000000	1.492373000000	0.477979000000
H	1.374726000000	1.152153000000	1.428489000000
C	2.228032000000	-1.332492000000	2.406594000000
H	1.143703000000	-1.286933000000	2.534145000000
H	2.508868000000	-2.387087000000	2.340477000000
H	2.680745000000	-0.912521000000	3.310721000000