

Supporting information for: Application of Classical Simulations for Computation of Vibrational Properties of Free Molecules

Denis Tikhonov,^{*,†,‡} Dmitry I. Sharapa,[¶] Jan Schwabdiessen,[†] and Vladimir V.
Rybkin[§]

*Universität Bielefeld, Lehrstuhl für Anorganische Chemie und Strukturchemie,
Universitätsstrasse 25, 33615, Bielefeld, Germany, M. V. Lomonosov Moscow State
University, Faculty of Chemistry, Department of Physical Chemistry, GSP-1, 1-3
Leninskiye Gory, 119991 Moscow, Russian Federation, Computer-Chemie-Centrum and
Interdisciplinary Center for Molecular Materials, Department Chemie und Pharmazie,
Friedrich-Alexander-Universität Erlangen-Nürnberg, 91052 Erlangen, Germany, and ETH
Zurich, Department of Materials, Wolfgang-Pauli-Strasse 27, CH-8093 Zurich, Switzerland*

E-mail: denis.tikhonov@uni-bielefeld.de

*To whom correspondence should be addressed

[†]UniBi

[‡]LMSU

[¶]FAU

[§]ETH

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UNEX input files used for obtaining the data in the article

Table S1 UNEX input file for BNZ.

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BASE=BASE,<base>,</base>
INT=INT,<INT>,</INT>

SMS=1-1,<sms_unex_ld>,</sms_unex_ld>
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;MOLXYZ=benz,XYZUNEX,<b_xyz_mp2>,</b_xyz_mp2>
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;AMPLITUDES=benz,FREEU,<b_md-cn-gle>,</b_md-cn-gle>
;AMPLITUDES=benz,FREEU,<b_md-gle>,</b_md-gle>
;AMPLITUDES=benz,FREEU,<b_md-gle-qa>,</b_md-gle-qa>
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;AMPLITUDES=benz,FREEU,<b_md-nh-qa>,</b_md-nh-qa>
;AMPLITUDES=benz,FREEU,<b_pimd>,</b_pimd>

GF=benz,AUTO,0.0487245

MINIMIZE=GEDINT+REGPRM,1-1,2-1

PRINT=GRAPHTERMS,benz

FUR=1-1,2-1
STOP

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molecules benz
FurTermDif=0.005
SMSModel=1
</base>

<benz>
formula C6H6
</benz>

<b_zmat_cc>
2 C
1 C 2 rCC
```

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10	C	7	rCC	3	120.0	1	0.0
6	C	10	rCC	7	120.0	3	0.0
4	H	2	rCH	1	120.0	3	180.0
12	H	1	rCH	3	120.0	7	180.0
5	H	3	rCH	7	120.0	10	180.0
9	H	7	rCH	10	120.0	6	180.0
11	H	10	rCH	6	120.0	2	180.0
8	H	6	rCH	2	120.0	1	180.0

Variables:

rCC 1.392

rCH 1.078

</b_zmat_cc>

; 3-X 25.03.2015 Short

; 4-X 02.04.2015 Long

<sms_unex_ld>

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</sms_unex_ld>

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24.60000000	0.14813767
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25.00000000	-0.26860488
25.20000000	-0.38518308
25.40000000	-0.52821552
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25.80000000	-0.54684238
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3.60000000	6.79093026
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6.40000000	4.68207702
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9.60000000	2.25176652
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13.80000000	1.35251845

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7.40000000	3.41563853
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9.20000000	2.59625528
9.40000000	2.53584162
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12.80000000	1.37362852

13.00000000	1.37997498
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21.80000000	0.61905391
22.00000000	0.61139674
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24.60000000	0.53256648
24.80000000	0.52286778
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27.60000000	0.45017370
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28.40000000	0.43214111
28.60000000	0.42650719
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29.00000000	0.41705979
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29.60000000	0.39880314
29.80000000	0.39258228
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30.80000000	0.36957582
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32.20000000 0.34471214
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<b_eldiff>

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C10	H11	1.0899	0.0752	-0.0161	67.0
C2	H4	1.0899	0.0752	-0.0161	67.0
C7	H9	1.0899	0.0752	-0.0161	67.0
C1	C2	1.4020	0.0460	-0.0068	8.7
C7	C10	1.4020	0.0460	-0.0068	8.7
C2	C6	1.4020	0.0460	-0.0068	8.7
C3	C7	1.4020	0.0460	-0.0068	8.7
C1	C3	1.4020	0.0460	-0.0068	8.7
C6	C10	1.4020	0.0460	-0.0068	8.7
C2	H12	2.1637	0.0980	-0.0134	17.5
C7	H11	2.1637	0.0980	-0.0134	17.5
C3	H9	2.1637	0.0980	-0.0134	17.5
H4	C6	2.1637	0.0980	-0.0134	17.5
C1	H4	2.1637	0.0980	-0.0133	17.1
C1	H5	2.1637	0.0980	-0.0133	17.1
H8	C10	2.1637	0.0980	-0.0133	17.1
H9	C10	2.1637	0.0980	-0.0133	17.1
C3	H12	2.1637	0.0980	-0.0133	17.1
C6	H11	2.1637	0.0980	-0.0133	17.1
C2	H8	2.1637	0.0980	-0.0134	17.5
H5	C7	2.1637	0.0980	-0.0134	17.5
C1	C6	2.4284	0.0550	-0.0094	3.5
C3	C10	2.4284	0.0550	-0.0094	3.5
C2	C3	2.4284	0.0550	-0.0094	3.5
C6	C7	2.4284	0.0550	-0.0094	3.5
C1	C7	2.4284	0.0550	-0.0094	3.5
C2	C10	2.4284	0.0550	-0.0094	3.5
H4	H8	2.4919	0.1588	-0.0123	-94.9
H5	H9	2.4919	0.1588	-0.0123	-94.9
H4	H12	2.4919	0.1588	-0.0122	-95.5
H5	H12	2.4919	0.1588	-0.0120	-96.1
H8	H11	2.4919	0.1588	-0.0120	-96.1
H9	H11	2.4919	0.1588	-0.0122	-95.5
C2	C7	2.8040	0.0613	-0.0101	0.8
C1	C10	2.8040	0.0613	-0.0101	0.8
C3	C6	2.8040	0.0613	-0.0101	0.8
C2	H5	3.4160	0.0940	-0.0161	37.7
C7	H8	3.4160	0.0940	-0.0161	37.7
C3	H11	3.4160	0.0940	-0.0161	38.0
C6	H12	3.4160	0.0940	-0.0161	38.0
C1	H8	3.4160	0.0940	-0.0161	38.0

C1	H9	3.4160	0.0940	-0.0161	38.0
H4	C10	3.4160	0.0940	-0.0161	38.0
H5	C10	3.4160	0.0940	-0.0161	38.0
C2	H11	3.4160	0.0940	-0.0161	37.7
C7	H12	3.4160	0.0940	-0.0161	37.7
C3	H4	3.4160	0.0940	-0.0161	37.7
C6	H9	3.4160	0.0940	-0.0161	37.7
C2	H9	3.8940	0.0933	-0.0169	53.9
H4	C7	3.8940	0.0933	-0.0169	53.9
C1	H11	3.8940	0.0933	-0.0169	53.9
C10	H12	3.8940	0.0933	-0.0169	53.9
C3	H8	3.8940	0.0933	-0.0169	53.9
H5	C6	3.8940	0.0933	-0.0169	53.9
H4	H11	4.3162	0.1287	-0.0203	12.5
H5	H11	4.3162	0.1287	-0.0204	12.8
H8	H12	4.3162	0.1287	-0.0204	12.8
H9	H12	4.3162	0.1287	-0.0203	12.5
H4	H5	4.3162	0.1287	-0.0202	12.2
H8	H9	4.3162	0.1287	-0.0202	12.2
H11	H12	4.9839	0.1170	-0.0221	106.9
H4	H9	4.9839	0.1170	-0.0222	106.9
H5	H8	4.9839	0.1170	-0.0221	106.9

</b_eldiff>

<b_md-cn-gle>

C1	H12	1.0899	0.0682	-0.0108	113.4
C10	H11	1.0899	0.0682	-0.0108	113.4
C3	H5	1.0899	0.0682	-0.0108	113.4
C6	H8	1.0899	0.0682	-0.0108	113.4
C7	H9	1.0899	0.0682	-0.0108	113.4
C2	H4	1.0899	0.0682	-0.0108	113.4
C3	C7	1.4020	0.0500	-0.0046	31.9
C2	C6	1.4020	0.0500	-0.0046	31.9
C6	C10	1.4020	0.0500	-0.0046	31.9
C1	C2	1.4020	0.0500	-0.0046	31.9
C7	C10	1.4020	0.0500	-0.0046	31.9
C1	C3	1.4020	0.0500	-0.0046	31.9
C3	H9	2.1637	0.0991	-0.0054	84.5
H4	C6	2.1637	0.0991	-0.0054	84.5
H5	C7	2.1637	0.0991	-0.0054	84.5
C2	H8	2.1637	0.0991	-0.0054	84.5
C2	H12	2.1637	0.0991	-0.0054	84.5
C3	H12	2.1637	0.0991	-0.0054	84.5
C7	H11	2.1637	0.0991	-0.0054	84.5
C6	H11	2.1637	0.0991	-0.0054	84.5
C1	H4	2.1637	0.0991	-0.0054	84.5
H8	C10	2.1637	0.0991	-0.0054	84.5
H9	C10	2.1637	0.0991	-0.0054	84.5

C1	H5	2.1637	0.0991	-0.0054	84.5
C6	C7	2.4284	0.0556	-0.0061	11.2
C2	C3	2.4284	0.0556	-0.0061	11.2
C2	C10	2.4284	0.0556	-0.0061	11.2
C1	C7	2.4284	0.0556	-0.0061	11.2
C3	C10	2.4284	0.0556	-0.0061	11.2
C1	C6	2.4284	0.0556	-0.0061	11.2
H4	H8	2.4919	0.1677	-0.0018	-16.6
H5	H9	2.4919	0.1677	-0.0018	-16.6
H8	H11	2.4919	0.1677	-0.0018	-16.6
H4	H12	2.4919	0.1677	-0.0018	-16.6
H9	H11	2.4919	0.1677	-0.0018	-16.6
H5	H12	2.4919	0.1677	-0.0018	-16.6
C2	C7	2.8040	0.0629	-0.0061	10.6
C3	C6	2.8040	0.0629	-0.0061	10.6
C1	C10	2.8040	0.0629	-0.0061	10.6
C2	H11	3.4160	0.0909	-0.0061	90.9
C6	H12	3.4160	0.0909	-0.0061	90.9
C7	H12	3.4160	0.0909	-0.0061	90.9
C3	H11	3.4160	0.0909	-0.0061	90.9
C2	H5	3.4160	0.0909	-0.0061	90.9
C6	H9	3.4160	0.0909	-0.0061	90.9
C7	H8	3.4160	0.0909	-0.0061	90.9
C3	H4	3.4160	0.0909	-0.0061	90.9
C1	H8	3.4160	0.0909	-0.0061	90.9
H4	C10	3.4160	0.0909	-0.0061	90.9
H5	C10	3.4160	0.0909	-0.0061	90.9
C1	H9	3.4160	0.0909	-0.0061	90.9
C3	H8	3.8940	0.0892	-0.0060	104.8
C2	H9	3.8940	0.0892	-0.0060	104.8
H4	C7	3.8940	0.0892	-0.0060	104.8
H5	C6	3.8940	0.0892	-0.0060	104.8
C1	H11	3.8940	0.0892	-0.0060	104.8
C10	H12	3.8940	0.0892	-0.0060	104.8
H5	H11	4.3162	0.1260	-0.0044	96.4
H9	H12	4.3162	0.1260	-0.0044	96.4
H8	H12	4.3162	0.1260	-0.0044	96.4
H4	H11	4.3162	0.1260	-0.0044	96.4
H4	H5	4.3162	0.1260	-0.0044	96.4
H8	H9	4.3162	0.1260	-0.0044	96.4
H11	H12	4.9839	0.1098	-0.0036	221.1
H5	H8	4.9839	0.1098	-0.0036	221.1
H4	H9	4.9839	0.1098	-0.0036	221.1

</b_md-cn-gle>

<b_md-gle>

C1	H12	1.0899	0.0300	-0.0019	4.7
C10	H11	1.0899	0.0300	-0.0019	4.7

C3	H5	1.0899	0.0300	-0.0019	4.7
C6	H8	1.0899	0.0300	-0.0019	4.7
C7	H9	1.0899	0.0300	-0.0019	4.7
C2	H4	1.0899	0.0300	-0.0019	4.7
C3	C7	1.4020	0.0283	-0.0074	4.9
C2	C6	1.4020	0.0283	-0.0074	4.9
C6	C10	1.4020	0.0283	-0.0074	4.9
C1	C2	1.4020	0.0283	-0.0074	4.9
C7	C10	1.4020	0.0283	-0.0074	4.9
C1	C3	1.4020	0.0283	-0.0074	4.9
C3	H9	2.1637	0.0544	-0.0048	1.2
H4	C6	2.1637	0.0544	-0.0048	1.2
H5	C7	2.1637	0.0544	-0.0048	1.2
C2	H8	2.1637	0.0544	-0.0048	1.2
C2	H12	2.1637	0.0544	-0.0048	1.2
C3	H12	2.1637	0.0544	-0.0048	1.2
C7	H11	2.1637	0.0544	-0.0048	1.2
C6	H11	2.1637	0.0544	-0.0048	1.2
C1	H4	2.1637	0.0544	-0.0048	1.2
H8	C10	2.1637	0.0544	-0.0048	1.2
H9	C10	2.1637	0.0544	-0.0048	1.2
C1	H5	2.1637	0.0544	-0.0048	1.2
C6	C7	2.4284	0.0404	-0.0103	2.2
C2	C3	2.4284	0.0404	-0.0103	2.2
C2	C10	2.4284	0.0404	-0.0103	2.2
C1	C7	2.4284	0.0404	-0.0103	2.2
C3	C10	2.4284	0.0404	-0.0103	2.2
C1	C6	2.4284	0.0404	-0.0103	2.2
H4	H8	2.4919	0.0990	-0.0035	-12.1
H5	H9	2.4919	0.0990	-0.0035	-12.1
H8	H11	2.4919	0.0990	-0.0035	-12.1
H4	H12	2.4919	0.0990	-0.0035	-12.1
H9	H11	2.4919	0.0990	-0.0035	-12.1
H5	H12	2.4919	0.0990	-0.0035	-12.1
C2	C7	2.8040	0.0496	-0.0109	-0.1
C3	C6	2.8040	0.0496	-0.0109	-0.1
C1	C10	2.8040	0.0496	-0.0109	-0.1
C2	H11	3.4160	0.0531	-0.0067	4.9
C6	H12	3.4160	0.0531	-0.0067	4.9
C7	H12	3.4160	0.0531	-0.0067	4.9
C3	H11	3.4160	0.0531	-0.0067	4.9
C2	H5	3.4160	0.0531	-0.0067	4.9
C6	H9	3.4160	0.0531	-0.0067	4.9
C7	H8	3.4160	0.0531	-0.0067	4.9
C3	H4	3.4160	0.0531	-0.0067	4.9
C1	H8	3.4160	0.0531	-0.0067	4.9
H4	C10	3.4160	0.0531	-0.0067	4.9
H5	C10	3.4160	0.0531	-0.0067	4.9

C1	H9	3.4160	0.0531	-0.0067	4.9
C3	H8	3.8940	0.0571	-0.0065	3.4
C2	H9	3.8940	0.0571	-0.0065	3.4
H4	C7	3.8940	0.0571	-0.0065	3.4
H5	C6	3.8940	0.0571	-0.0065	3.4
C1	H11	3.8940	0.0571	-0.0065	3.4
C10	H12	3.8940	0.0571	-0.0065	3.4
H5	H11	4.3162	0.0700	-0.0028	-0.3
H9	H12	4.3162	0.0700	-0.0028	-0.3
H8	H12	4.3162	0.0700	-0.0028	-0.3
H4	H11	4.3162	0.0700	-0.0028	-0.3
H4	H5	4.3162	0.0700	-0.0028	-0.3
H8	H9	4.3162	0.0700	-0.0028	-0.3
H11	H12	4.9839	0.0640	-0.0010	1.6
H5	H8	4.9839	0.0640	-0.0010	1.6
H4	H9	4.9839	0.0640	-0.0010	1.6

</b_md-gle>

<b_md-gle-qa>

C1	H12	1.0899	0.0754	-0.0121	68.4
C10	H11	1.0899	0.0754	-0.0121	68.4
C3	H5	1.0899	0.0754	-0.0121	68.4
C6	H8	1.0899	0.0754	-0.0121	68.4
C7	H9	1.0899	0.0754	-0.0121	68.4
C2	H4	1.0899	0.0754	-0.0121	68.4
C3	C7	1.4020	0.0471	-0.0102	9.9
C2	C6	1.4020	0.0471	-0.0102	9.9
C6	C10	1.4020	0.0471	-0.0102	9.9
C1	C2	1.4020	0.0471	-0.0102	9.9
C7	C10	1.4020	0.0471	-0.0102	9.9
C1	C3	1.4020	0.0471	-0.0102	9.9
C3	H9	2.1637	0.1044	-0.0014	3.2
H4	C6	2.1637	0.1044	-0.0014	3.2
H5	C7	2.1637	0.1044	-0.0014	3.2
C2	H8	2.1637	0.1044	-0.0014	3.2
C2	H12	2.1637	0.1044	-0.0014	3.2
C3	H12	2.1637	0.1044	-0.0014	3.2
C7	H11	2.1637	0.1044	-0.0014	3.2
C6	H11	2.1637	0.1044	-0.0014	3.2
C1	H4	2.1637	0.1044	-0.0014	3.2
H8	C10	2.1637	0.1044	-0.0014	3.2
H9	C10	2.1637	0.1044	-0.0014	3.2
C1	H5	2.1637	0.1044	-0.0014	3.2
C6	C7	2.4284	0.0575	-0.0095	-0.7
C2	C3	2.4284	0.0575	-0.0095	-0.7
C2	C10	2.4284	0.0575	-0.0095	-0.6
C1	C7	2.4284	0.0575	-0.0095	-0.6
C3	C10	2.4284	0.0575	-0.0095	-0.6

C1	C6	2.4284	0.0575	-0.0095	-0.6
H4	H8	2.4919	0.1641	0.0045	-33.0
H5	H9	2.4919	0.1641	0.0045	-33.0
H8	H11	2.4919	0.1641	0.0045	-33.0
H4	H12	2.4919	0.1641	0.0045	-33.0
H9	H11	2.4919	0.1641	0.0045	-33.0
H5	H12	2.4919	0.1641	0.0045	-33.0
C2	C7	2.8040	0.0641	-0.0099	-3.7
C3	C6	2.8040	0.0641	-0.0099	-3.7
C1	C10	2.8040	0.0641	-0.0099	-3.7
C2	H11	3.4160	0.1030	-0.0063	18.5
C6	H12	3.4160	0.1030	-0.0063	18.5
C7	H12	3.4160	0.1030	-0.0063	18.5
C3	H11	3.4160	0.1030	-0.0063	18.5
C2	H5	3.4160	0.1030	-0.0063	18.5
C6	H9	3.4160	0.1030	-0.0063	18.5
C7	H8	3.4160	0.1030	-0.0063	18.5
C3	H4	3.4160	0.1030	-0.0063	18.5
C1	H8	3.4160	0.1030	-0.0063	18.5
H4	C10	3.4160	0.1030	-0.0063	18.5
H5	C10	3.4160	0.1030	-0.0063	18.5
C1	H9	3.4160	0.1030	-0.0063	18.5
C3	H8	3.8940	0.1067	-0.0054	10.1
C2	H9	3.8940	0.1067	-0.0054	10.1
H4	C7	3.8940	0.1067	-0.0054	10.1
H5	C6	3.8940	0.1067	-0.0054	10.1
C1	H11	3.8940	0.1067	-0.0054	10.1
C10	H12	3.8940	0.1067	-0.0054	10.1
H5	H11	4.3162	0.1382	0.0006	-2.1
H9	H12	4.3162	0.1382	0.0006	-2.1
H8	H12	4.3162	0.1382	0.0006	-2.1
H4	H11	4.3162	0.1382	0.0006	-2.1
H4	H5	4.3162	0.1382	0.0006	-2.1
H8	H9	4.3162	0.1382	0.0006	-2.1
H11	H12	4.9839	0.1314	0.0010	9.6
H5	H8	4.9839	0.1314	0.0010	9.6
H4	H9	4.9839	0.1314	0.0010	9.6

</b_md-gle-qa>

<b_md-nh>

C1	H12	1.0899	0.0217	0.0004	1.0
C10	H11	1.0899	0.0217	0.0004	1.0
C3	H5	1.0899	0.0217	0.0004	1.0
C6	H8	1.0899	0.0217	0.0004	1.0
C7	H9	1.0899	0.0217	0.0004	1.0
C2	H4	1.0899	0.0217	0.0004	1.0
C3	C7	1.4020	0.0242	-0.0003	2.6
C2	C6	1.4020	0.0242	-0.0003	2.6

C6	C10	1.4020	0.0242	-0.0003	2.6
C1	C2	1.4020	0.0242	-0.0003	2.6
C7	C10	1.4020	0.0242	-0.0003	2.6
C1	C3	1.4020	0.0242	-0.0003	2.6
C3	H9	2.1637	0.0473	0.0027	-3.6
H4	C6	2.1637	0.0473	0.0027	-3.6
H5	C7	2.1637	0.0473	0.0027	-3.6
C2	H8	2.1637	0.0473	0.0027	-3.6
C2	H12	2.1637	0.0473	0.0027	-3.6
C3	H12	2.1637	0.0473	0.0027	-3.6
C7	H11	2.1637	0.0473	0.0027	-3.6
C6	H11	2.1637	0.0473	0.0027	-3.6
C1	H4	2.1637	0.0473	0.0027	-3.6
H8	C10	2.1637	0.0473	0.0027	-3.6
H9	C10	2.1637	0.0473	0.0027	-3.6
C1	H5	2.1637	0.0473	0.0027	-3.6
C6	C7	2.4284	0.0430	0.0013	0.4
C2	C3	2.4284	0.0430	0.0013	0.4
C2	C10	2.4284	0.0430	0.0013	0.4
C1	C7	2.4284	0.0430	0.0013	0.4
C3	C10	2.4284	0.0430	0.0013	0.4
C1	C6	2.4284	0.0430	0.0013	0.4
H4	H8	2.4919	0.0883	0.0048	-28.9
H5	H9	2.4919	0.0883	0.0048	-28.9
H8	H11	2.4919	0.0883	0.0048	-28.9
H4	H12	2.4919	0.0883	0.0048	-28.9
H9	H11	2.4919	0.0883	0.0048	-28.9
H5	H12	2.4919	0.0883	0.0048	-28.9
C2	C7	2.8040	0.0585	0.0023	-6.2
C3	C6	2.8040	0.0585	0.0023	-6.2
C1	C10	2.8040	0.0585	0.0023	-6.2
C2	H11	3.4160	0.0488	0.0052	1.7
C6	H12	3.4160	0.0488	0.0052	1.7
C7	H12	3.4160	0.0488	0.0052	1.7
C3	H11	3.4160	0.0488	0.0052	1.7
C2	H5	3.4160	0.0488	0.0052	1.7
C6	H9	3.4160	0.0488	0.0052	1.7
C7	H8	3.4160	0.0488	0.0052	1.7
C3	H4	3.4160	0.0488	0.0052	1.7
C1	H8	3.4160	0.0488	0.0052	1.7
H4	C10	3.4160	0.0488	0.0052	1.7
H5	C10	3.4160	0.0488	0.0052	1.7
C1	H9	3.4160	0.0488	0.0052	1.7
C3	H8	3.8940	0.0620	0.0067	-3.5
C2	H9	3.8940	0.0620	0.0067	-3.5
H4	C7	3.8940	0.0620	0.0067	-3.5
H5	C6	3.8940	0.0620	0.0067	-3.5
C1	H11	3.8940	0.0620	0.0067	-3.5

C10	H12	3.8940	0.0620	0.0067	-3.5
H5	H11	4.3162	0.0609	0.0093	-7.3
H9	H12	4.3162	0.0609	0.0093	-7.3
H8	H12	4.3162	0.0609	0.0093	-7.3
H4	H11	4.3162	0.0609	0.0093	-7.3
H4	H5	4.3162	0.0609	0.0093	-7.3
H8	H9	4.3162	0.0609	0.0093	-7.3
H11	H12	4.9839	0.0658	0.0117	-1.0
H5	H8	4.9839	0.0658	0.0117	-1.0
H4	H9	4.9839	0.0658	0.0117	-1.0

</b_md-nh>

<b_md-nh-qa>

C1	H12	1.0899	0.0759	-0.0065	50.4
C10	H11	1.0899	0.0759	-0.0065	50.4
C3	H5	1.0899	0.0759	-0.0065	50.4
C6	H8	1.0899	0.0759	-0.0065	50.4
C7	H9	1.0899	0.0759	-0.0065	50.4
C2	H4	1.0899	0.0759	-0.0065	50.4
C3	C7	1.4020	0.0467	-0.0054	12.7
C2	C6	1.4020	0.0467	-0.0054	12.7
C6	C10	1.4020	0.0467	-0.0054	12.7
C1	C2	1.4020	0.0467	-0.0054	12.7
C7	C10	1.4020	0.0467	-0.0054	12.7
C1	C3	1.4020	0.0467	-0.0054	12.7
C3	H9	2.1637	0.1083	0.0105	-33.3
H4	C6	2.1637	0.1083	0.0105	-33.3
H5	C7	2.1637	0.1083	0.0105	-33.3
C2	H8	2.1637	0.1083	0.0105	-33.3
C2	H12	2.1637	0.1083	0.0105	-33.3
C3	H12	2.1637	0.1083	0.0105	-33.3
C7	H11	2.1637	0.1083	0.0105	-33.3
C6	H11	2.1637	0.1083	0.0105	-33.3
C1	H4	2.1637	0.1083	0.0105	-33.3
H8	C10	2.1637	0.1083	0.0105	-33.3
H9	C10	2.1637	0.1083	0.0105	-33.3
C1	H5	2.1637	0.1083	0.0105	-33.3
C6	C7	2.4284	0.0599	0.0019	0.5
C2	C3	2.4284	0.0599	0.0019	0.5
C2	C10	2.4284	0.0599	0.0019	0.5
C1	C7	2.4284	0.0599	0.0019	0.5
C3	C10	2.4284	0.0599	0.0019	0.5
C1	C6	2.4284	0.0599	0.0019	0.5
H4	H8	2.4919	0.1690	0.0181	-133.3
H5	H9	2.4919	0.1690	0.0181	-133.3
H8	H11	2.4919	0.1690	0.0181	-133.3
H4	H12	2.4919	0.1690	0.0181	-133.3
H9	H11	2.4919	0.1690	0.0181	-133.3

H5	H12	2.4919	0.1690	0.0181	-133.3
C2	C7	2.8040	0.0663	0.0029	-4.4
C3	C6	2.8040	0.0663	0.0029	-4.4
C1	C10	2.8040	0.0663	0.0029	-4.4
C2	H11	3.4160	0.1117	0.0065	17.6
C6	H12	3.4160	0.1117	0.0065	17.6
C7	H12	3.4160	0.1117	0.0065	17.6
C3	H11	3.4160	0.1117	0.0065	17.6
C2	H5	3.4160	0.1117	0.0065	17.6
C6	H9	3.4160	0.1117	0.0065	17.6
C7	H8	3.4160	0.1117	0.0065	17.6
C3	H4	3.4160	0.1117	0.0065	17.6
C1	H8	3.4160	0.1117	0.0065	17.6
H4	C10	3.4160	0.1117	0.0065	17.6
H5	C10	3.4160	0.1117	0.0065	17.6
C1	H9	3.4160	0.1117	0.0065	17.6
C3	H8	3.8940	0.1245	0.0109	-17.5
C2	H9	3.8940	0.1245	0.0109	-17.5
H4	C7	3.8940	0.1245	0.0109	-17.5
H5	C6	3.8940	0.1245	0.0109	-17.5
C1	H11	3.8940	0.1245	0.0109	-17.5
C10	H12	3.8940	0.1245	0.0109	-17.5
H5	H11	4.3162	0.1422	0.0167	-59.0
H9	H12	4.3162	0.1422	0.0167	-59.0
H8	H12	4.3162	0.1422	0.0167	-59.0
H4	H11	4.3162	0.1422	0.0167	-59.0
H4	H5	4.3162	0.1422	0.0167	-59.0
H8	H9	4.3162	0.1422	0.0167	-59.0
H11	H12	4.9839	0.1503	0.0147	13.4
H5	H8	4.9839	0.1503	0.0147	13.4
H4	H9	4.9839	0.1503	0.0147	13.4

</b_md-nh-qa>

<b_pimd>

C1	H12	1.0899	0.0770	-0.0131	76.8
C10	H11	1.0899	0.0770	-0.0131	76.8
C3	H5	1.0899	0.0770	-0.0131	76.8
C6	H8	1.0899	0.0770	-0.0131	76.8
C7	H9	1.0899	0.0770	-0.0131	76.8
C2	H4	1.0899	0.0770	-0.0131	76.8
C3	C7	1.4020	0.0464	-0.0040	9.2
C2	C6	1.4020	0.0464	-0.0040	9.2
C6	C10	1.4020	0.0464	-0.0040	9.2
C1	C2	1.4020	0.0464	-0.0040	9.2
C7	C10	1.4020	0.0464	-0.0040	9.2
C1	C3	1.4020	0.0464	-0.0040	9.2
C3	H9	2.1637	0.0993	-0.0084	26.5
H4	C6	2.1637	0.0993	-0.0084	26.5

H5	C7	2.1637	0.0993	-0.0084	26.5
C2	H8	2.1637	0.0993	-0.0084	26.5
C2	H12	2.1637	0.0993	-0.0084	26.5
C3	H12	2.1637	0.0993	-0.0084	26.5
C7	H11	2.1637	0.0993	-0.0084	26.5
C6	H11	2.1637	0.0993	-0.0084	26.5
C1	H4	2.1637	0.0993	-0.0084	26.5
H8	C10	2.1637	0.0993	-0.0084	26.5
H9	C10	2.1637	0.0993	-0.0084	26.5
C1	H5	2.1637	0.0993	-0.0084	26.5
C6	C7	2.4284	0.0553	-0.0047	2.5
C2	C3	2.4284	0.0553	-0.0047	2.5
C2	C10	2.4284	0.0553	-0.0047	2.5
C1	C7	2.4284	0.0553	-0.0047	2.5
C3	C10	2.4284	0.0553	-0.0047	2.5
C1	C6	2.4284	0.0553	-0.0047	2.5
H4	H8	2.4919	0.1604	-0.0064	-60.7
H5	H9	2.4919	0.1604	-0.0064	-60.7
H8	H11	2.4919	0.1604	-0.0064	-60.7
H4	H12	2.4919	0.1604	-0.0064	-60.7
H9	H11	2.4919	0.1604	-0.0064	-60.7
H5	H12	2.4919	0.1604	-0.0064	-60.7
C2	C7	2.8040	0.0605	-0.0047	-7.0
C3	C6	2.8040	0.0605	-0.0047	-7.0
C1	C10	2.8040	0.0605	-0.0047	-7.0
C2	H11	3.4160	0.0953	-0.0086	41.7
C6	H12	3.4160	0.0953	-0.0086	41.7
C7	H12	3.4160	0.0953	-0.0086	41.7
C3	H11	3.4160	0.0953	-0.0086	41.7
C2	H5	3.4160	0.0953	-0.0086	41.7
C6	H9	3.4160	0.0953	-0.0086	41.7
C7	H8	3.4160	0.0953	-0.0086	41.7
C3	H4	3.4160	0.0953	-0.0086	41.7
C1	H8	3.4160	0.0953	-0.0086	41.7
H4	C10	3.4160	0.0953	-0.0086	41.7
H5	C10	3.4160	0.0953	-0.0086	41.7
C1	H9	3.4160	0.0953	-0.0086	41.7
C3	H8	3.8940	0.0939	-0.0084	50.3
C2	H9	3.8940	0.0939	-0.0084	50.3
H4	C7	3.8940	0.0939	-0.0084	50.3
H5	C6	3.8940	0.0939	-0.0084	50.3
C1	H11	3.8940	0.0939	-0.0084	50.3
C10	H12	3.8940	0.0939	-0.0084	50.3
H5	H11	4.3162	0.1301	-0.0103	22.4
H9	H12	4.3162	0.1301	-0.0103	22.4
H8	H12	4.3162	0.1301	-0.0103	22.4
H4	H11	4.3162	0.1301	-0.0103	22.4
H4	H5	4.3162	0.1301	-0.0103	22.4

H8	H9	4.3162	0.1301	-0.0103	22.4
H11	H12	4.9839	0.1188	-0.0105	97.1
H5	H8	4.9839	0.1188	-0.0105	97.1
H4	H9	4.9839	0.1188	-0.0105	97.1

</b_pimd>

;Benzene @ B3LYP/cc-pVTZ

<b_xyz_b3lyp>

RENUM=1-1,2-2,3-6,4-10,5-7,6-3,7-12,8-4

RENUM=9-8,10-11,11-9,12-5

C	0.6954261899	1.2045134939	0.0000000000
C	-0.6954261899	1.2045134939	0.0000000000
C	-1.3908523799	0.0000000000	0.0000000000
C	-0.6954261899	-1.2045134939	0.0000000000
C	0.6954261899	-1.2045134939	0.0000000000
C	1.3908523799	0.0000000000	0.0000000000
H	1.2364027647	2.1415124071	0.0000000000
H	-1.2364027647	2.1415124071	0.0000000000
H	-2.4728055294	0.0000000000	0.0000000000
H	-1.2364027647	-2.1415124071	0.0000000000
H	1.2364027647	-2.1415124071	0.0000000000
H	2.4728055294	0.0000000000	0.0000000000

</b_xyz_b3lyp>

;Benzene @ BP86/cc-pVTZ

<b_xyz_bp86>

RENUM=1-1,2-2,3-6,4-10,5-7,6-3,7-12,8-4

RENUM=9-8,10-11,11-9,12-5

C	0.6992781545	1.2111852922	0.0000000000
C	-0.6992781545	1.2111852922	0.0000000000
C	-1.3985563090	0.0000000000	0.0000000000
C	-0.6992781545	-1.2111852922	0.0000000000
C	0.6992781545	-1.2111852922	0.0000000000
C	1.3985563090	0.0000000000	0.0000000000
H	1.2447753056	2.1560140732	0.0000000000
H	-1.2447753056	2.1560140732	0.0000000000
H	-2.4895506111	0.0000000000	0.0000000000
H	-1.2447753056	-2.1560140732	0.0000000000
H	1.2447753056	-2.1560140732	0.0000000000
H	2.4895506111	0.0000000000	0.0000000000

</b_xyz_bp86>

;Benzene @ MP2/cc-pVTZ

<b_xyz_mp2>

RENUM=1-1,2-2,3-6,4-10,5-7,6-3,7-12,8-4

RENUM=9-8,10-11,11-9,12-5

C	0.6966648356	1.2066588910	0.0000000000
---	--------------	--------------	--------------

C	-0.6966648356	1.2066588910	0.0000000000
C	-1.3933296711	0.0000000000	0.0000000000
C	-0.6966648356	-1.2066588910	0.0000000000
C	0.6966648356	-1.2066588910	0.0000000000
C	1.3933296711	0.0000000000	0.0000000000
H	1.2374293457	2.1432904975	0.0000000000
H	-1.2374293457	2.1432904975	0.0000000000
H	-2.4748586913	0.0000000000	0.0000000000
H	-1.2374293457	-2.1432904975	0.0000000000
H	1.2374293457	-2.1432904975	0.0000000000
H	2.4748586913	0.0000000000	0.0000000000

</b_xyz_mp2>

;Benzene @ PBE0/cc-pVTZ

<b_xyz_pbe0>

RENUM=1-1,2-2,3-6,4-10,5-7,6-3,7-12,8-4

RENUM=9-8,10-11,11-9,12-5

C	0.6938611770	1.2018028120	0.0000000000
C	-0.6938611770	1.2018028120	0.0000000000
C	-1.3877223540	0.0000000000	0.0000000000
C	-0.6938611770	-1.2018028120	0.0000000000
C	0.6938611770	-1.2018028120	0.0000000000
C	1.3877223540	0.0000000000	0.0000000000
H	1.2356357158	2.1401838394	0.0000000000
H	-1.2356357158	2.1401838394	0.0000000000
H	-2.4712714315	0.0000000000	0.0000000000
H	-1.2356357158	-2.1401838394	0.0000000000
H	1.2356357158	-2.1401838394	0.0000000000
H	2.4712714315	0.0000000000	0.0000000000

</b_xyz_pbe0>

Table S2 UNEX input file for CMTC.

```
BASE=BASE,<base>,</base>

INT=INT,<INT>,</INT>
SMS=2-1,<sms_ld>,</sms_ld>
SMS=1-1,<sms_sd>,</sms_sd>

;CCSD(T)
MOLXYZ=gauche,XYZUNEX,<gauche_ccsdt_xyz>,</gauche_ccsdt_xyz>
MOLXYZ=anti,XYZUNEX,<anti_ccsdt_xyz>,</anti_ccsdt_xyz>

;MP2
;MOLXYZ=gauche,XYZUNEX,<gauche_mp2_xyz>,</gauche_mp2_xyz>
;MOLXYZ=anti,XYZUNEX,<anti_mp2_xyz>,</anti_mp2_xyz>

;DFT GEOM-S
;B3LYP
;MOLXYZ=gauche,XYZUNEX,<gauche_b3lyp_xyz>,</gauche_b3lyp_xyz>
;MOLXYZ=anti,XYZUNEX,<anti_b3lyp_xyz>,</anti_b3lyp_xyz>

;PBE0
;MOLXYZ=gauche,XYZUNEX,<gauche_pbe0_xyz>,</gauche_pbe0_xyz>
;MOLXYZ=anti,XYZUNEX,<anti_pbe0_xyz>,</anti_pbe0_xyz>

;BP86
;MOLXYZ=gauche,XYZUNEX,<gauche_bp86_xyz>,</gauche_bp86_xyz>
;MOLXYZ=anti,XYZUNEX,<anti_bp86_xyz>,</anti_bp86_xyz>

;VM
;AMPLITUDES=gauche,FREEU,<gauche_amp_vm>,</gauche_amp_vm>
;AMPLITUDES=anti,FREEU,<anti_amp_vm>,</anti_amp_vm>

;MD-QA
;AMPLITUDES=gauche,FREEU,<gauche_amp_md-qa>,</gauche_amp_md-qa>
;AMPLITUDES=anti,FREEU,<anti_amp_md-qa>,</anti_amp_md-qa>

;MD
AMPLITUDES=gauche,FREEU,<gauche_amp_md>,</gauche_amp_md>
AMPLITUDES=anti,FREEU,<anti_amp_md>,</anti_amp_md>

GF=gauche,AUTO,0.0484505
GF=anti,AUTO,0.0484505

MINIMIZE=GEDINT+REGPRM,1-1,2-1,1000,2000

PRINT=GRAPHTERMS,gauche
```

PRINT=GRAPHTERMS,anti

FUR=1-1,2-1

STOP

<base>

molecules gauche, anti

FurType=modern

FurDamp=0.001

FurTermDif=0.005

SMSModel=1

</base>

<gauche>

formula C2H2ClNS

amount 0.85

</gauche>

<anti>

formula C2H2ClNS

</anti>

<INT>

INT1 NtoP=250.0 StoP=4.5 Lam=0.048478 VarSc=1000

6.40000000	0.88152774
6.60000000	0.91941711
6.80000000	0.95150490
7.00000000	0.98028843
7.20000000	1.00542154
7.40000000	1.01280022
7.60000000	1.01467203
7.80000000	1.01238815
8.00000000	1.01261783
8.20000000	1.00795669
8.40000000	1.00763814
8.60000000	1.01200051
8.80000000	1.00902724
9.00000000	1.00367530
9.20000000	0.98986108
9.40000000	0.97463726
9.60000000	0.95962469
9.80000000	0.94971030
10.00000000	0.95280889
10.20000000	0.96588752
10.40000000	0.98696816
10.60000000	1.01252770
10.80000000	1.04126583

11.00000000	1.06275746
11.20000000	1.07519031
11.40000000	1.07852027
11.60000000	1.07507434
11.80000000	1.06907784
12.00000000	1.06135391
12.20000000	1.05663904
12.40000000	1.05216254
12.60000000	1.04834284
12.80000000	1.04636698
13.00000000	1.04561240
13.20000000	1.04491976
13.40000000	1.04574278
13.60000000	1.04650451
13.80000000	1.04892518
14.00000000	1.05058687
14.20000000	1.05510585
14.40000000	1.06035333
14.60000000	1.06925084
14.80000000	1.07646675
15.00000000	1.08440753
15.20000000	1.08812883
15.40000000	1.08884032
15.60000000	1.08584721
15.80000000	1.08302619
16.00000000	1.07810058
16.20000000	1.07349502
16.40000000	1.07165463
16.60000000	1.07296029
16.80000000	1.07468883
17.00000000	1.07822123
17.20000000	1.08354176
17.40000000	1.08798520
17.60000000	1.09397494
17.80000000	1.09656684
18.00000000	1.09725658
18.20000000	1.09906980
18.40000000	1.09952538
18.60000000	1.10036418
18.80000000	1.10139977
19.00000000	1.09956715
19.20000000	1.09855312
19.40000000	1.09476601
19.60000000	1.09119221
19.80000000	1.08623721
20.00000000	1.08301627
20.20000000	1.08042795
20.40000000	1.07851854

20.60000000	1.08032187
20.80000000	1.08208133
21.00000000	1.08448171
21.20000000	1.08749660
21.40000000	1.09184468
21.60000000	1.09421299
21.80000000	1.09563498
22.00000000	1.09854377
22.20000000	1.09956578
22.40000000	1.09952471
22.60000000	1.09807739
22.80000000	1.09691271
23.00000000	1.09494882
23.20000000	1.09350513
23.40000000	1.09058666
23.60000000	1.08746770
23.80000000	1.08635188
24.00000000	1.08339544
24.20000000	1.08176093
24.40000000	1.08185183
24.60000000	1.08140197
24.80000000	1.08201093
25.00000000	1.08195617
25.20000000	1.08196501
25.40000000	1.08123153
25.60000000	1.08095794
25.80000000	1.08007140
26.00000000	1.07810981
26.20000000	1.07811546
26.40000000	1.07822544
26.60000000	1.07798185
26.80000000	1.07826536
27.00000000	1.07879598
27.20000000	1.07914073
27.40000000	1.07994719
27.60000000	1.08090875
27.80000000	1.08077176
28.00000000	1.07995094
28.20000000	1.08154082
28.40000000	1.08115494
28.60000000	1.08108565
28.80000000	1.08292570
29.00000000	1.08316655
29.20000000	1.08343232
29.40000000	1.08407003
29.60000000	1.08205384
29.80000000	1.08142473
30.00000000	1.08117998

30.20000000	1.07812220
30.40000000	1.07761157
30.60000000	1.07787869
30.80000000	1.07809572
31.00000000	1.07879968
31.20000000	1.07838088
31.40000000	1.07829481
31.60000000	1.07905563
31.80000000	1.07943098
32.00000000	1.07873702
32.20000000	1.08007366
INT2 NtoP=500.0 StoP=4.5 Lam=0.048423 VarSc=2000	
2.20000000	0.61292309
2.40000000	0.63690834
2.60000000	0.66147127
2.80000000	0.66770615
3.00000000	0.67589980
3.20000000	0.68225140
3.40000000	0.69678549
3.60000000	0.72635642
3.80000000	0.76379511
4.00000000	0.81267316
4.20000000	0.86000742
4.40000000	0.90806983
4.60000000	0.94226187
4.80000000	0.95347454
5.00000000	0.94589999
5.20000000	0.92553753
5.40000000	0.89497063
5.60000000	0.86216876
5.80000000	0.84133125
6.00000000	0.83539317
6.20000000	0.84826838
6.40000000	0.86848883
6.60000000	0.89546453
6.80000000	0.92655951
7.00000000	0.95315946
7.20000000	0.97212524
7.40000000	0.98161351
7.60000000	0.98228619
7.80000000	0.97724676
8.00000000	0.97254576
8.20000000	0.97020749
8.40000000	0.97097280
8.60000000	0.97353377
8.80000000	0.97291521
9.00000000	0.96437448
9.20000000	0.95239391

9.40000000	0.93537398
9.60000000	0.92003894
9.80000000	0.91105381
10.00000000	0.90947075
10.20000000	0.92198855
10.40000000	0.94276195
10.60000000	0.97100487
10.80000000	0.99815774
11.00000000	1.02266803
11.20000000	1.03753093
11.40000000	1.04326827
11.60000000	1.04142343
11.80000000	1.03492742
12.00000000	1.02658089
12.20000000	1.01757141
12.40000000	1.01038898
12.60000000	1.00607192
12.80000000	1.00436231
13.00000000	1.00285796
13.20000000	1.00206094
13.40000000	1.00116951
13.60000000	1.00072781
13.80000000	1.00020339
14.00000000	1.00204154
14.20000000	1.00411037
14.40000000	1.00834426
14.60000000	1.01587287
14.80000000	1.02271652
15.00000000	1.02948982
15.20000000	1.03240555
15.40000000	1.03150372
15.60000000	1.02955883
15.80000000	1.02362510
16.00000000	1.01652723
16.20000000	1.00982219
16.40000000	1.00487829
16.60000000	1.00363891
16.80000000	1.00280986
17.00000000	1.00634915
17.20000000	1.01247230
17.40000000	1.01601190

</INT>

<sms_ld>

2.20000000	-0.17812766
2.40000000	-0.17629725
2.60000000	-0.16996088
2.80000000	-0.21056515

3.00000000	-0.24754855
3.20000000	-0.29135578
3.40000000	-0.30868579
3.60000000	-0.26966029
3.80000000	-0.19205946
4.00000000	-0.05641543
4.20000000	0.09005320
4.40000000	0.25678019
4.60000000	0.37754895
4.80000000	0.40085189
5.00000000	0.33437520
5.20000000	0.19884164
5.40000000	0.00172524
5.60000000	-0.21731107
5.80000000	-0.37653665
6.00000000	-0.45087825
6.20000000	-0.40726940
6.40000000	-0.30839830
6.60000000	-0.15500922
6.80000000	0.03741625
7.00000000	0.20954760
7.20000000	0.33478707
7.40000000	0.39388096
7.60000000	0.38547041
7.80000000	0.32814112
8.00000000	0.26695331
8.20000000	0.21924339
8.40000000	0.19348728
8.60000000	0.18130064
8.80000000	0.14106254
9.00000000	0.02915415
9.20000000	-0.11718540
9.40000000	-0.31438855
9.60000000	-0.50059850
9.80000000	-0.62918170
10.00000000	-0.68634639
10.20000000	-0.60017954
10.40000000	-0.42366634
10.60000000	-0.16059004
10.80000000	0.10097733
11.00000000	0.34333007
11.20000000	0.48668553
11.40000000	0.53158907
11.60000000	0.49107405
11.80000000	0.39600213
12.00000000	0.27798056
12.20000000	0.15073714
12.40000000	0.04443043

12.60000000	-0.02744209
12.80000000	-0.06700076
13.00000000	-0.10406278
13.20000000	-0.13178160
13.40000000	-0.16024363
13.60000000	-0.18187438
13.80000000	-0.20359534
14.00000000	-0.19120058
14.20000000	-0.17364069
14.40000000	-0.12329379
14.60000000	-0.02273547
14.80000000	0.07111077
15.00000000	0.16739144
15.20000000	0.20919661
15.40000000	0.19556070
15.60000000	0.16810448
15.80000000	0.08010360
16.00000000	-0.02588712
16.20000000	-0.12623120
16.40000000	-0.19940263
16.60000000	-0.21308442
16.80000000	-0.22104261
17.00000000	-0.15614772
17.20000000	-0.04623448
17.40000000	0.02132396

</sms_ld>

<sms_sd>

6.40000000	-0.33229707
6.60000000	-0.12802462
6.80000000	0.04980662
7.00000000	0.21534678
7.20000000	0.36416840
7.40000000	0.38976992
7.60000000	0.37460098
7.80000000	0.32598686
8.00000000	0.29500541
8.20000000	0.22274928
8.40000000	0.18410065
8.60000000	0.18482953
8.80000000	0.12229585
9.00000000	0.03700472
9.20000000	-0.12812015
9.40000000	-0.31154837
9.60000000	-0.49827147
9.80000000	-0.64004002
10.00000000	-0.65448301
10.20000000	-0.56459834

10.40000000	-0.38493716
10.60000000	-0.14816865
10.80000000	0.13406830
11.00000000	0.34860157
11.20000000	0.47024218
11.40000000	0.49244686
11.60000000	0.43622198
11.80000000	0.34704418
12.00000000	0.23319855
12.20000000	0.15156474
12.40000000	0.06983183
12.60000000	-0.00636859
12.80000000	-0.06129965
13.00000000	-0.10182676
13.20000000	-0.14239059
13.40000000	-0.16331848
13.60000000	-0.18494474
13.80000000	-0.18334406
14.00000000	-0.19116569
14.20000000	-0.15739083
14.40000000	-0.11091223
14.60000000	-0.00865855
14.80000000	0.07261989
15.00000000	0.16796704
15.20000000	0.20265361
15.40000000	0.19276700
15.60000000	0.12565299
15.80000000	0.06034802
16.00000000	-0.03940680
16.20000000	-0.13550823
16.40000000	-0.18753378
16.60000000	-0.18729433
16.80000000	-0.17842646
17.00000000	-0.13706615
17.20000000	-0.06235318
17.40000000	0.00042776
17.60000000	0.09341716
17.80000000	0.12957811
18.00000000	0.13376228
18.20000000	0.15979833
18.40000000	0.16262022
18.60000000	0.17371921
18.80000000	0.18979090
19.00000000	0.15271060
19.20000000	0.13148598
19.40000000	0.05683161
19.60000000	-0.01456727
19.80000000	-0.11437719

20.00000000	-0.18133930
20.20000000	-0.23678873
20.40000000	-0.27943777
20.60000000	-0.24632859
20.80000000	-0.21320476
21.00000000	-0.16551722
21.20000000	-0.10322558
21.40000000	-0.01031123
21.60000000	0.04277391
21.80000000	0.07760413
22.00000000	0.14729951
22.20000000	0.17799236
22.40000000	0.18703787
22.60000000	0.16597312
22.80000000	0.15232272
23.00000000	0.12123192
23.20000000	0.10269012
23.40000000	0.05017945
23.60000000	-0.00730712
23.80000000	-0.01764240
24.00000000	-0.07204446
24.20000000	-0.09531288
24.40000000	-0.07704297
24.60000000	-0.07214760
24.80000000	-0.04147873
25.00000000	-0.02763150
25.20000000	-0.01282644
25.40000000	-0.01763382
25.60000000	-0.01186186
25.80000000	-0.02304989
26.00000000	-0.06374788
26.20000000	-0.05506781
26.40000000	-0.04510269
26.60000000	-0.04602927
26.80000000	-0.03453144
27.00000000	-0.01790215
27.20000000	-0.00774269
27.40000000	0.01372916
27.60000000	0.03862293
27.80000000	0.03254389
28.00000000	0.00675276
28.20000000	0.04834179
28.40000000	0.03439635
28.60000000	0.02939509
28.80000000	0.07947329
29.00000000	0.08414979
29.20000000	0.08997286
29.40000000	0.10721763

29.60000000	0.04658203
29.80000000	0.02688061
30.00000000	0.01891323
30.20000000	-0.07359365
30.40000000	-0.08941758
30.60000000	-0.08117106
30.80000000	-0.07385499
31.00000000	-0.05087455
31.20000000	-0.06227164
31.40000000	-0.06322321
31.60000000	-0.03746887
31.80000000	-0.02377669
32.00000000	-0.04428054
32.20000000	0.00034631

</sms_sd>

<anti_b3lyp_xyz>

C	0.1390085500	-0.1135347107	0.0000000000
S	1.9758996010	0.0749113986	0.0000000000
C	2.0343780742	1.7693577043	0.0000000000
N	2.0960366136	2.9239134007	0.0000000000
Cl	-0.2235372107	-1.8571189780	0.0000000000
H	-0.2755060180	0.3296419564	0.8972948767
H	-0.2755060180	0.3296419564	-0.8972948767

</anti_b3lyp_xyz>

<anti_bp86_xyz>

C	0.1303532636	-0.1149119713	0.0000000000
S	1.9766594640	0.0745486306	0.0000000000
C	2.0368702611	1.7695824897	0.0000000000
N	2.1037930368	2.9386496818	0.0000000000
Cl	-0.2246840695	-1.8624437579	0.0000000000
H	-0.2848561557	0.3322596728	0.9065320607
H	-0.2848561557	0.3322596728	-0.9065320607

</anti_bp86_xyz>

<anti_ccsdt_xyz>

C	-0.5313885258	0.6954708898	0.0000000000
S	0.5482684374	-0.7820938442	0.0000000000
C	2.0218707349	0.0646497333	0.0000000000
N	3.0350503826	0.6385697873	0.0000000000
Cl	-2.2075588646	0.1249481218	-0.0000000000
H	-0.3568566000	1.2762531604	-0.8944503636
H	-0.3568566000	1.2762531604	0.8944503636

</anti_ccsdt_xyz>

<anti_mp2_xyz>

C	0.1626952889	-0.1020134442	0.0000000000
---	--------------	---------------	--------------

S	1.9825585667	0.0482862816	0.0000000000
C	2.0213264323	1.7402103744	0.0000000000
N	2.0476004633	2.9166700226	0.0000000000
Cl	-0.2157084315	-1.8250853269	0.0000000000
H	-0.2437696980	0.3514822832	0.8966398787
H	-0.2437696980	0.3514822832	-0.8966398787

</anti_mp2_xyz>

<anti_pbe0_xyz>

C	0.1492237493	-0.1117173784	0.0000000000
S	1.9684571624	0.0657437682	0.0000000000
C	2.0249309671	1.7511347420	0.0000000000
N	2.0797975673	2.9054906900	0.0000000000
Cl	-0.2111284215	-1.8361616765	0.0000000000
H	-0.2644879970	0.3371320744	0.8979062765
H	-0.2644879970	0.3371320744	-0.8979062765

</anti_pbe0_xyz>

<gauche_b3lyp_xyz>

C	-0.0039745391	0.0393810320	-0.0026382383
S	1.8195708777	0.0212148230	-0.0083202903
C	2.1378119288	1.6860667684	0.0327483161
N	2.4081680978	2.8087885417	0.0680643401
Cl	-0.7636062550	0.4600738878	-1.5694252433
H	-0.3621140072	0.7369288429	0.7443163758
H	-0.2921769646	-0.9761756236	0.2491663392

</gauche_b3lyp_xyz>

<gauche_bp86_xyz>

C	-0.0096515117	0.0433128598	-0.0027542874
S	1.8219170006	0.0216231006	-0.0096692505
C	2.1449940195	1.6863429105	0.0389982643
N	2.4278910211	2.8209252119	0.0787139859
Cl	-0.7739284088	0.4529864078	-1.5749396301
H	-0.3649857067	0.7546388684	0.7461879538
H	-0.2975402763	-0.9796557315	0.2604183581

</gauche_bp86_xyz>

<gauche_ccsdt_xyz>

C	-0.7538412793	-0.6343392960	0.6847995763
S	0.7628216230	-1.0543623667	-0.2165387537
C	1.5853121252	0.4175008322	-0.0063475971
N	2.1789912382	1.4102249866	0.1221611412
Cl	-1.8038417917	0.5255045092	-0.1542379322
H	-0.4988296597	-0.2276480937	1.6530478454
H	-1.2881220179	-1.5698513399	0.7924763911

</gauche_ccsdt_xyz>

```

<gauche_mp2_xyz>
C      0.0089357979   0.0039561737  -0.0009799406
S      1.8189362980  -0.0219484271   0.0111456231
C      2.0731222918   1.6501189862  -0.0104041145
N      2.2805910999   2.8079046163  -0.0219135442
Cl     -0.6945399532   0.5279884826  -1.5364096663
H      -0.3504960912   0.6580074273   0.7850641477
H      -0.2909544450  -1.0223031714   0.1895798799
</gauche_mp2_xyz>

```

```

<gauche_pbe0_xyz>
C      0.0028150604   0.0380637071  -0.0078089061
S      1.8108788089   0.0157503356  -0.0092536442
C      2.1173419461   1.6740414630   0.0204819317
N      2.3737779864   2.7997066892   0.0478732424
Cl     -0.7375517358   0.4737171352  -1.5543941921
H      -0.3538904589   0.7267571688   0.7516510560
H      -0.2879592693  -0.9809790864   0.2380657855
</gauche_pbe0_xyz>

```

```

<anti_amp_md>
C1      H6      1.0975   0.0425  -0.0060    1.19e+00
C1      H7      1.0975   0.0425  -0.0060    1.19e+00
C3      N4      1.1625   0.0134  -0.0008   -1.40e-04
S2      C3      1.6918   0.0197  -0.0023   -1.21e-02
C1     C15      1.7614   0.0099  -0.0011    1.98e-03
H6      H7      1.8065   0.1107  -0.0026    1.54e+01
C1      S2      1.8347   0.0312  -0.0087    3.89e-02
C15     H7      2.3645   0.0621  -0.0012    3.42e+00
C15     H6      2.3645   0.0621  -0.0012    3.42e+00
S2      H6      2.4361   0.0634  -0.0039    4.69e+00
S2      H7      2.4361   0.0634  -0.0039    4.69e+00
C1      C3      2.6667   0.0445   0.0145   -8.49e+00
S2      N4      2.8542   0.0207  -0.0012   -1.40e-02
C3      H7      2.8606   0.1722   0.0262    2.11e+02
C3      H6      2.8606   0.1722   0.0262    2.11e+02
S2     C15      2.9024   0.0284  -0.0272    1.29e+00
C1      N4      3.6190   0.0615   0.0369   -2.74e+01
N4      H7      3.6282   0.2255   0.0561    7.14e+02
N4      H6      3.6282   0.2255   0.0561    7.14e+02
C3     C15      4.2484   0.0401   0.0242   -5.06e+00
N4     C15      5.2999   0.0549   0.0571   -1.41e+01
</anti_amp_md>

```

```

<gauche_amp_md>
C1      H6      1.0971   0.0345  -0.0051    5.64e-01
C1      H7      1.0990   0.0386  -0.0053    6.98e-01
C3      N4      1.1616   0.0118  -0.0010   -3.18e-03

```

S2	C3	1.6926	0.0191	-0.0012	1.18e-01
C1	C15	1.7660	0.0168	-0.0031	-6.57e-02
H6	H7	1.7953	0.1075	-0.0033	2.09e-01
C1	S2	1.8146	0.0352	-0.0131	2.14e-01
S2	H7	2.3414	0.0781	-0.0222	-4.07e+00
C15	H6	2.3617	0.0690	-0.0040	-2.07e-01
C15	H7	2.3659	0.0704	0.0011	5.37e+00
S2	H6	2.4163	0.0727	-0.0070	4.24e+00
C1	C3	2.6916	0.0570	-0.0122	-3.89e+00
C3	H6	2.8075	0.2083	0.0233	4.02e+02
S2	N4	2.8533	0.0209	0.0007	8.08e-02
S2	C15	3.0210	0.0529	-0.0028	6.93e-01
C3	C15	3.4390	0.3408	-0.0586	-1.77e+03
N4	H6	3.5868	0.2709	0.0387	7.41e+02
C3	H7	3.6168	0.0906	0.0432	-3.28e+01
C1	N4	3.6722	0.0968	-0.0025	-4.18e+01
N4	C15	4.1624	0.5023	-0.0507	-7.31e+03
N4	H7	4.6721	0.1224	0.0750	-1.28e+02

</gauche_amp_md>

<anti_amp_md-qa>

C1	H6	1.0975	0.0763	-0.0060	3.53282e+00
C1	H7	1.0975	0.0763	-0.0060	3.53282e+00
C3	N4	1.1625	0.0339	0.0001	-5.30713e-03
S2	C3	1.6918	0.0419	-0.0010	-1.25155e-01
C1	C15	1.7614	0.0417	-0.0009	1.62802e-01
H6	H7	1.8065	0.1285	-0.0015	9.19211e+00
C1	S2	1.8347	0.0532	-0.0066	-7.37922e-01
C15	H7	2.3645	0.0990	-0.0027	7.40019e+00
C15	H6	2.3645	0.0990	-0.0027	7.40019e+00
S2	H6	2.4361	0.1012	-0.0067	1.02220e+01
S2	H7	2.4361	0.1012	-0.0067	1.02220e+01
C1	C3	2.6667	0.0769	0.0416	-5.37994e+01
S2	N4	2.8542	0.0441	-0.0003	-1.16037e-01
C3	H7	2.8606	0.2054	0.0218	2.37707e+02
C3	H6	2.8606	0.2054	0.0218	2.37707e+02
S2	C15	2.9024	0.1022	0.0927	-7.21494e+02
C1	N4	3.6190	0.1243	0.0590	-1.31329e+02
N4	H7	3.6282	0.2563	0.0490	8.14430e+02
N4	H6	3.6282	0.2563	0.0490	8.14430e+02
C3	C15	4.2484	0.0752	0.0266	-3.12672e+00
N4	C15	5.2999	0.1450	0.0072	4.72221e+02

</anti_amp_md-qa>

<gauche_amp_md-qa>

C1	H6	1.0971	0.0764	-0.0054	3.80026e+00
C1	H7	1.0990	0.0766	-0.0047	3.04911e+00
C3	N4	1.1616	0.0339	0.0004	-8.19420e-02

S2	C3	1.6926	0.0429	-0.0042	1.09769e+00
C1	C15	1.7660	0.0497	0.0039	-2.25262e+00
H6	H7	1.7953	0.1322	0.0000	-7.33766e-02
C1	S2	1.8146	0.0575	-0.0100	-1.86855e+00
S2	H7	2.3414	0.1143	-0.0150	-1.27005e+01
C15	H6	2.3617	0.1079	-0.0008	-5.59546e-01
C15	H7	2.3659	0.1065	-0.0004	9.55471e+00
S2	H6	2.4163	0.1113	-0.0070	7.39784e+00
C1	C3	2.6916	0.0869	-0.0056	-1.39898e+01
C3	H6	2.8075	0.2068	0.0235	2.21087e+02
S2	N4	2.8533	0.0460	-0.0008	7.61300e-01
S2	C15	3.0210	0.0768	-0.0026	2.35339e+00
C3	C15	3.4390	0.3700	-0.0450	-2.66173e+03
N4	H6	3.5868	0.2414	0.0406	3.10726e+02
C3	H7	3.6168	0.1219	0.0471	-1.01574e+01
C1	N4	3.6722	0.1249	0.0081	-9.14920e+01
N4	C15	4.1624	0.3833	-0.1083	-3.08555e+03
N4	H7	4.6721	0.1391	0.0761	-3.04455e+00

</gauche_amp_md-qa>

<anti_amp_vm>

C1	H6	1.0975	0.0758	-0.0139	0.0000
C1	H7	1.0975	0.0758	-0.0174	0.0000
C3	N4	1.1625	0.0338	-0.0038	0.0000
S2	C3	1.6918	0.0445	-0.0058	0.0000
C1	C15	1.7614	0.0497	-0.0096	0.0000
H6	H7	1.8065	0.1225	-0.0182	0.0000
C1	S2	1.8347	0.0539	-0.0112	0.0000
C15	H6	2.3645	0.1082	-0.0215	0.0000
C15	H7	2.3645	0.1082	0.0023	0.0000
S2	H6	2.4361	0.1107	-0.0073	0.0000
S2	H7	2.4361	0.1107	-0.0225	0.0000
C1	C3	2.6667	0.0960	-0.0236	0.0000
S2	N4	2.8542	0.0476	-0.0011	0.0000
C3	H6	2.8606	0.2744	0.3455	0.0000
C3	H7	2.8606	0.2744	-0.3868	0.0000
S2	C15	2.9024	0.0868	-0.0297	0.0000
C1	N4	3.6190	0.1487	0.0305	0.0000
N4	H7	3.6282	0.3730	-0.4421	0.0000
N4	H6	3.6282	0.3729	0.5393	0.0000
C3	C15	4.2484	0.0894	0.0173	0.0000
N4	C15	5.2999	0.1313	0.0841	0.0000

</anti_amp_vm>

<gauche_amp_vm>

C1	H6	1.0971	0.0757	-0.0160	0.0000
C1	H7	1.0990	0.0759	-0.0154	0.0000
C3	N4	1.1616	0.0337	-0.0037	0.0000

S2	C3	1.6926	0.0445	-0.0060	0.0000
C1	C15	1.7660	0.0510	-0.0085	0.0000
H6	H7	1.7953	0.1238	-0.0176	0.0000
C1	S2	1.8146	0.0539	-0.0105	0.0000
S2	H7	2.3414	0.1156	-0.0181	0.0000
C15	H6	2.3617	0.1076	-0.0138	0.0000
C15	H7	2.3659	0.1084	-0.0100	0.0000
S2	H6	2.4163	0.1100	-0.0142	0.0000
C1	C3	2.6916	0.0898	-0.0155	0.0000
C3	H6	2.8075	0.2076	0.0162	0.0000
S2	N4	2.8533	0.0478	-0.0002	0.0000
S2	C15	3.0210	0.0749	-0.0131	0.0000
C3	C15	3.4390	0.2139	-0.0614	0.0000
N4	H6	3.5868	0.2961	0.0257	0.0000
C3	H7	3.6168	0.1123	-0.0037	0.0000
C1	N4	3.6722	0.1530	-0.0227	0.0000
N4	C15	4.1624	0.3266	-0.1021	0.0000
N4	H7	4.6721	0.1516	0.0018	0.0000

</gauche_amp_vm>

Table S3 UNEX input file for PZA.

```
BASE=BASE,<base>,</base>
INT=INT,<INT>,</INT>

SMS=1-1,<sms_ld>,</sms_ld>
SMS=2-1,<sms_sd>,</sms_sd>

MOLXYZ=pza,XYZUNEX,<pza_mp2_xyz>,</pza_mp2_xyz>

;DFT geometries
;MOLXYZ=pza,XYZUNEX,<pza_bp86_xyz>,</pza_bp86_xyz>
;MOLXYZ=pza,XYZUNEX,<pza_b3lyp_xyz>,</pza_b3lyp_xyz>
;MOLXYZ=pza,XYZUNEX,<pza_pbe0_xyz>,</pza_pbe0_xyz>

;AMPLITUDES=pza,FREEU,<pza_bp86_md_amp>,</pza_bp86_md_amp>
;AMPLITUDES=pza,FREEU,<pza_bp86_md-qa_amp>,</pza_bp86_md-qa_amp>
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PRINT=GRAPHTERMS,pza

FUR=1-1,2-1

STOP

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C4	H11	1.1063	0.0314	-0.0039	2.8
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C4	N5	1.3450	0.0251	-0.0026	2.3
C1	N2	1.3490	0.0253	-0.0026	2.7
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C3	C4	1.4101	0.0277	-0.0032	3.7
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H13	H14	1.7861	0.0581	0.0127	-5.0
C7	H13	2.0655	0.0615	-0.0021	-0.1
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N5	H11	2.0961	0.0494	-0.0020	10.0
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C4	H10	2.1955	0.0586	-0.0058	3.5

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C1	O9	2.4077	0.0510	-0.0035	-4.4
C1	N8	2.4089	0.0496	-0.0202	-13.4
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N2	C6	2.4099	0.0292	-0.0020	0.5
C3	N5	2.4116	0.0316	-0.0015	0.4
N2	C7	2.4717	0.0556	-0.0067	-14.3
C1	H13	2.5075	0.1217	-0.0297	-151.2
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H10	H11	2.5443	0.0962	-0.0098	7.3
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O9	H14	2.5782	0.0836	0.0158	-29.8
C1	C4	2.6845	0.0351	-0.0076	0.1
C3	C6	2.6892	0.0337	-0.0042	-1.1
N2	N8	2.7072	0.1185	-0.0372	-251.0
C7	H12	2.7306	0.1188	-0.0183	-148.7
N2	N5	2.8286	0.0366	0.0007	-6.5
C6	O9	2.8709	0.1282	-0.0149	-319.4
O9	H13	3.1981	0.0555	0.0087	-19.5
C6	H11	3.2818	0.0481	-0.0034	6.7
C4	H12	3.2887	0.0536	-0.0033	5.1
C1	H10	3.2889	0.0528	-0.0049	17.1
C1	H14	3.3611	0.0513	0.0012	-23.7
N2	H12	3.3967	0.0513	-0.0061	5.8
N2	H11	3.3995	0.0485	-0.0032	1.7
N5	H10	3.4092	0.0545	-0.0026	11.0
C3	H13	3.5428	0.2178	-0.0595	-1118.9
N2	O9	3.5935	0.0520	0.0073	2.3
C3	C7	3.6894	0.0474	-0.0074	1.0
C6	N8	3.7078	0.0506	-0.0059	-11.6
N2	H14	3.7257	0.1245	-0.0159	-373.2
N5	C7	3.7841	0.0542	-0.0066	-12.6
C1	H11	3.7907	0.0465	-0.0055	2.8
C3	H12	3.7923	0.0523	-0.0044	-1.3
C6	H10	3.7950	0.0513	-0.0035	4.3
C6	H13	3.9161	0.1206	-0.0125	-236.3
H10	H13	3.9644	0.2527	-0.0699	-998.3
C3	N8	4.0497	0.1256	-0.0298	-361.6
N8	H12	4.0686	0.1115	-0.0020	-60.2
H11	H12	4.1926	0.0725	0.0015	20.4
C4	C7	4.2039	0.0454	-0.0079	12.4
N5	O9	4.2146	0.1329	-0.0076	-345.1
H12	H13	4.5148	0.1202	-0.0007	73.3
C7	H10	4.5659	0.0757	-0.0040	11.8

C6	H14	4.5751	0.0686	0.0163	-107.8
C4	H13	4.6428	0.1952	-0.0394	-797.5
N8	H10	4.6696	0.1683	-0.0322	-694.2
C3	09	4.6951	0.0634	0.0071	-23.3
H12	H14	4.7748	0.1507	0.0190	-692.0
N5	H13	4.8166	0.1568	-0.0167	-440.0
N5	N8	4.8184	0.0609	-0.0041	-63.8
H10	H12	4.8983	0.0643	-0.0029	8.4
C4	N8	4.9285	0.0936	-0.0171	-222.0
C4	09	4.9421	0.1046	0.0004	-185.9
C3	H14	5.0682	0.1322	-0.0073	-558.9
C7	H11	5.3103	0.0552	-0.0038	12.1
H11	H13	5.6547	0.2112	-0.0386	-1132.2
H10	H14	5.6558	0.1884	-0.0109	-1320.7
09	H10	5.6570	0.0732	0.0151	35.6
N5	H14	5.7566	0.0595	0.0203	-59.0
C4	H14	5.9373	0.0882	0.0077	-197.3
N8	H11	6.0053	0.1079	-0.0126	-357.2
09	H11	6.0274	0.1171	0.0062	-236.0
H11	H14	7.0197	0.1041	0.0141	-376.0

</pza_bp86_md_amp>

<pza_bp86_md-qa_amp>

N8	H14	1.0210	0.0728	-0.0016	7.9
N8	H13	1.0239	0.0733	0.0004	0.8
C6	H12	1.1037	0.0768	-0.0047	14.8
C3	H10	1.1060	0.0768	-0.0086	37.4
C4	H11	1.1063	0.0769	-0.0059	31.0
C7	09	1.2314	0.0385	-0.0012	1.3
N2	C3	1.3426	0.0439	-0.0062	8.6
N5	C6	1.3439	0.0439	-0.0059	9.1
C4	N5	1.3450	0.0443	-0.0054	7.7
C1	N2	1.3490	0.0441	-0.0058	8.3
C7	N8	1.3657	0.0447	-0.0108	6.7
C3	C4	1.4101	0.0462	-0.0064	9.7
C1	C6	1.4120	0.0455	-0.0093	11.8
C1	C7	1.5201	0.0505	-0.0082	5.4
H13	H14	1.7861	0.1266	0.0211	-17.3
C7	H13	2.0655	0.1113	0.0021	-1.0
C7	H14	2.0674	0.1092	0.0216	-102.2
N2	H10	2.0956	0.0945	-0.0032	28.1
N5	H11	2.0961	0.0987	-0.0046	53.2
N5	H12	2.1078	0.0941	0.0001	27.5
C1	H12	2.1790	0.0954	-0.0102	22.4
C3	H11	2.1913	0.1025	-0.0041	22.3
C4	H10	2.1955	0.0972	-0.0037	6.7
N2	H13	2.2553	0.1995	-0.0653	-1164.8
C4	C6	2.2830	0.0515	-0.0043	-1.0

C1	C3	2.2899	0.0511	-0.0071	4.9
N8	O9	2.3064	0.0500	-0.0039	2.1
N2	C4	2.4026	0.0534	-0.0043	6.5
C1	O9	2.4077	0.0640	-0.0023	-5.0
C1	N8	2.4089	0.0671	-0.0156	-41.4
C1	N5	2.4096	0.0525	-0.0058	6.8
N2	C6	2.4099	0.0521	-0.0018	1.9
C3	N5	2.4116	0.0514	-0.0012	1.1
N2	C7	2.4717	0.0678	-0.0049	-15.1
C1	H13	2.5075	0.1532	-0.0223	-220.9
C6	C7	2.5346	0.0745	-0.0076	-33.6
H10	H11	2.5443	0.1587	-0.0037	6.2
O9	H12	2.5604	0.2142	-0.0307	-970.0
O9	H14	2.5782	0.1347	0.0229	-59.7
C1	C4	2.6845	0.0564	-0.0063	-2.2
C3	C6	2.6892	0.0558	-0.0024	-3.6
N2	N8	2.7072	0.1191	-0.0370	-322.9
C7	H12	2.7306	0.1540	-0.0110	-184.4
N2	N5	2.8286	0.0606	0.0058	-20.7
C6	O9	2.8709	0.1190	-0.0170	-195.0
O9	H13	3.1981	0.1064	0.0192	-84.4
C6	H11	3.2818	0.0964	-0.0055	35.4
C4	H12	3.2887	0.0901	-0.0032	13.2
C1	H10	3.2889	0.0908	-0.0091	49.1
C1	H14	3.3611	0.1093	0.0204	-171.6
N2	H12	3.3967	0.0884	-0.0065	15.0
N2	H11	3.3995	0.0971	-0.0022	8.6
N5	H10	3.4092	0.0919	-0.0044	29.4
C3	H13	3.5428	0.2167	-0.0598	-1092.5
N2	O9	3.5935	0.0637	0.0074	2.9
C3	C7	3.6894	0.0638	-0.0069	0.0
C6	N8	3.7078	0.0672	-0.0037	-16.6
N2	H14	3.7257	0.1813	0.0018	-773.0
N5	C7	3.7841	0.0697	-0.0046	-16.8
C1	H11	3.7907	0.0950	-0.0053	13.1
C3	H12	3.7923	0.0878	-0.0026	-4.1
C6	H10	3.7950	0.0887	-0.0037	12.1
C6	H13	3.9161	0.1514	-0.0057	-227.3
H10	H13	3.9644	0.2653	-0.0668	-1412.1
C3	N8	4.0497	0.1181	-0.0316	-268.9
N8	H12	4.0686	0.1445	0.0017	-63.1
H11	H12	4.1926	0.1297	-0.0000	69.8
C4	C7	4.2039	0.0641	-0.0100	18.3
N5	O9	4.2146	0.1260	-0.0090	-226.0
H12	H13	4.5148	0.1729	0.0001	108.0
C7	H10	4.5659	0.1111	-0.0037	17.9
C6	H14	4.5751	0.1212	0.0417	-371.8
C4	H13	4.6428	0.1989	-0.0386	-569.8

N8	H10	4.6696	0.1759	-0.0305	-435.4
C3	09	4.6951	0.0732	0.0083	-20.8
H12	H14	4.7748	0.2034	0.0355	-885.2
N5	H13	4.8166	0.1763	-0.0130	-328.5
N5	N8	4.8184	0.0784	0.0020	-96.5
H10	H12	4.8983	0.1144	-0.0033	27.8
C4	N8	4.9285	0.1041	-0.0139	-240.6
C4	09	4.9421	0.1034	0.0001	-123.6
C3	H14	5.0682	0.1854	0.0113	-1012.1
C7	H11	5.3103	0.1030	-0.0072	48.4
H11	H13	5.6547	0.2399	-0.0325	-978.0
H10	H14	5.6558	0.2324	0.0019	-1313.3
09	H10	5.6570	0.1078	0.0121	61.6
N5	H14	5.7566	0.1168	0.0376	-214.1
C4	H14	5.9373	0.1442	0.0322	-563.0
N8	H11	6.0053	0.1466	0.0016	-447.8
09	H11	6.0274	0.1511	0.0135	-254.4
H11	H14	7.0197	0.1691	0.0464	-981.3

</pza_bp86_md-qa_amp>

<pza_bp86_eldiff_amp>

N8	H14	1.0210	0.0491	-0.0217	56.2
N8	H13	1.0239	0.0602	-0.0201	59.3
C6	H12	1.1037	0.0740	-0.0169	65.8
C3	H10	1.1060	0.0745	-0.0173	68.2
C4	H11	1.1063	0.0737	-0.0171	67.9
C7	09	1.2314	0.0351	-0.0035	4.9
N2	C3	1.3426	0.0439	-0.0066	8.9
N5	C6	1.3439	0.0437	-0.0057	8.9
C4	N5	1.3450	0.0435	-0.0057	9.2
C1	N2	1.3490	0.0444	-0.0062	9.4
C7	N8	1.3657	0.0403	-0.0139	8.5
C3	C4	1.4101	0.0455	-0.0073	10.1
C1	C6	1.4120	0.0462	-0.0082	10.0
C1	C7	1.5201	0.0521	-0.0093	17.0
H13	H14	1.7861	0.1082	0.0021	40.0
C7	H13	2.0655	0.0992	-0.0094	38.3
C7	H14	2.0674	0.0928	0.0051	-6.0
N2	H10	2.0956	0.0955	-0.0116	17.3
N5	H11	2.0961	0.0944	-0.0127	18.9
N5	H12	2.1078	0.0949	-0.0052	14.4
C1	H12	2.1790	0.0990	-0.0258	35.9
C3	H11	2.1913	0.0965	-0.0193	24.2
C4	H10	2.1955	0.0972	-0.0200	27.3
N2	H13	2.2553	0.2070	-0.0497	2376.7
C4	C6	2.2830	0.0535	-0.0130	3.1
C1	C3	2.2899	0.0540	-0.0137	3.3
N8	09	2.3064	0.0452	-0.0086	4.4

N2	C4	2.4026	0.0533	-0.0074	3.8
C1	O9	2.4077	0.0617	-0.0057	15.7
C1	N8	2.4089	0.0643	-0.0253	28.6
C1	N5	2.4096	0.0539	-0.0070	3.8
N2	C6	2.4099	0.0538	-0.0059	4.2
C3	N5	2.4116	0.0530	-0.0049	3.9
N2	C7	2.4717	0.0645	-0.0084	17.5
C1	H13	2.5075	0.1629	-0.0290	586.3
C6	C7	2.5346	0.0705	-0.0184	31.1
H10	H11	2.5443	0.1587	-0.0299	-49.3
O9	H12	2.5604	0.1918	-0.0557	876.7
O9	H14	2.5782	0.1418	0.0200	-137.3
C1	C4	2.6845	0.0595	-0.0147	1.9
C3	C6	2.6892	0.0592	-0.0116	1.6
N2	N8	2.7072	0.1058	-0.0348	274.6
C7	H12	2.7306	0.1459	-0.0419	206.8
N2	N5	2.8286	0.0638	0.0002	-2.5
C6	O9	2.8709	0.1094	-0.0224	119.6
O9	H13	3.1981	0.0853	0.0004	27.0
C6	H11	3.2818	0.0906	-0.0183	42.1
C4	H12	3.2887	0.0908	-0.0139	41.3
C1	H10	3.2889	0.0921	-0.0182	42.7
C1	H14	3.3611	0.0871	-0.0040	49.0
N2	H12	3.3967	0.0932	-0.0205	42.0
N2	H11	3.3995	0.0915	-0.0174	40.6
N5	H10	3.4092	0.0920	-0.0161	41.3
C3	H13	3.5428	0.2148	-0.0479	2749.6
N2	O9	3.5935	0.0630	0.0006	13.0
C3	C7	3.6894	0.0657	-0.0135	16.4
C6	N8	3.7078	0.0684	-0.0206	17.6
N2	H14	3.7257	0.1254	-0.0152	284.8
N5	C7	3.7841	0.0691	-0.0141	25.0
C1	H11	3.7907	0.0906	-0.0217	56.0
C3	H12	3.7923	0.0910	-0.0191	54.0
C6	H10	3.7950	0.0912	-0.0192	56.4
C6	H13	3.9161	0.1621	-0.0232	444.1
H10	H13	3.9644	0.2462	-0.0518	3092.4
C3	N8	4.0497	0.1092	-0.0314	241.6
N8	H12	4.0686	0.1412	-0.0355	100.9
H11	H12	4.1926	0.1247	-0.0131	12.4
C4	C7	4.2039	0.0689	-0.0167	15.1
N5	O9	4.2146	0.1111	-0.0177	91.0
H12	H13	4.5148	0.1781	-0.0329	202.3
C7	H10	4.5659	0.1088	-0.0126	6.3
C6	H14	4.5751	0.1033	0.0039	-23.5
C4	H13	4.6428	0.2045	-0.0383	1994.2
N8	H10	4.6696	0.1612	-0.0306	176.3
C3	O9	4.6951	0.0718	-0.0050	12.8

H12	H14	4.7748	0.1836	-0.0114	-111.9
N5	H13	4.8166	0.1844	-0.0220	976.0
N5	N8	4.8184	0.0748	-0.0157	26.2
H10	H12	4.8983	0.1148	-0.0240	108.9
C4	N8	4.9285	0.0921	-0.0257	107.0
C4	O9	4.9421	0.0946	-0.0129	39.9
C3	H14	5.0682	0.1298	-0.0092	201.7
C7	H11	5.3103	0.0976	-0.0205	69.5
H11	H13	5.6547	0.2233	-0.0453	2329.0
H10	H14	5.6558	0.1891	-0.0090	-14.0
O9	H10	5.6570	0.1053	-0.0016	35.9
N5	H14	5.7566	0.0980	0.0107	30.8
C4	H14	5.9373	0.1072	0.0000	101.0
N8	H11	6.0053	0.1205	-0.0290	160.0
O9	H11	6.0274	0.1211	-0.0146	78.1
H11	H14	7.0197	0.1333	-0.0012	137.5

</pza_bp86_eldiff_amp>

;PZA @ B3LYP/cc-pVTZ

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N	0.4031263743	-1.1876453774	0.0000000000
C	1.7324971655	-1.2129415492	0.0000000000
C	2.4812771951	-0.0406594780	0.0000000000
N	1.9089419325	1.1619528179	0.0000000000
C	0.5782097697	1.1863846146	0.0000000000
C	-1.6830987953	0.0926199076	0.0000000000
N	-2.3010424555	-1.1092454559	0.0000000000
O	-2.2600397986	1.1661471247	0.0000000000
H	2.2123353740	-2.1841053218	0.0000000000
H	3.5642155330	-0.0739995375	0.0000000000
H	0.0822306501	2.1470565707	0.0000000000
H	-1.7532893744	-1.9523237111	0.0000000000
H	-3.3046708786	-1.1416477785	0.0000000000

</pza_b3lyp_xyz>

;PZA @ BP86/cc-pVTZ

<pza_bp86_xyz>

C	-0.1796449173	0.0149304214	0.0000000000
N	0.3988434250	-1.1991755142	0.0000000000
C	1.7381747674	-1.2211120901	0.0000000000
C	2.4922427726	-0.0429353282	0.0000000000
N	1.9219077361	1.1719989672	0.0000000000
C	0.5812156494	1.1926721846	0.0000000000
C	-1.6905590968	0.0958561158	0.0000000000
N	-2.3013118603	-1.1185325463	0.0000000000
O	-2.2767616436	1.1777282300	0.0000000000
H	2.2206067129	-2.2017957231	0.0000000000

H	3.5847452829	-0.0773903280	0.0000000000
H	0.0797037991	2.1617396596	0.0000000000
H	-1.7316927574	-1.9591204954	0.0000000000
H	-3.3126929982	-1.1652149482	0.0000000000

</pza_bp86_xyz>

;PZA @ MP2/cc-pVTZ

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C	-0.1791017509	0.0111229112	0.0000000000
N	0.3913153685	-1.2018284607	0.0000000000
C	1.7285421796	-1.2142417652	0.0000000000
C	2.4775856477	-0.0409529077	0.0000000000
N	1.9100122074	1.1722511772	0.0000000000
C	0.5724756463	1.1857958913	0.0000000000
C	-1.6802100020	0.0948929191	0.0000000000
N	-2.2857999967	-1.1110959132	0.0000000000
O	-2.2562147793	1.1734992228	0.0000000000
H	2.2116181429	-2.1826114191	0.0000000000
H	3.5591687020	-0.0764530059	0.0000000000
H	0.0706427769	2.1428216725	0.0000000000
H	-1.7206556341	-1.9417445588	0.0000000000
H	-3.2882598086	-1.1533769085	0.0000000000

</pza_mp2_xyz>

;PZA @ PBE0/cc-pVTZ

<pza_pbe0_xyz>

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N	0.3981046778	-1.1864882236	0.0000000000
C	1.7231706327	-1.2101360513	0.0000000000
C	2.4701829587	-0.0396595111	0.0000000000
N	1.9020533463	1.1601869768	0.0000000000
C	0.5755243065	1.1826628639	0.0000000000
C	-1.6770952423	0.0931893460	0.0000000000
N	-2.2868193945	-1.1061643781	0.0000000000
O	-2.2505261687	1.1643700396	0.0000000000
H	2.2049420039	-2.1822137030	0.0000000000
H	3.5548158082	-0.0743459522	0.0000000000
H	0.0745675904	2.1431692704	0.0000000000
H	-1.7296968685	-1.9426573318	0.0000000000
H	-3.2891960912	-1.1450044509	0.0000000000

</pza_pbe0_xyz>

Table S4 UNEX input file for ICB.

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;MOLXYZ=mol,XYZUNEX,<icarb_pbe0_xyz>,</icarb_pbe0_xyz>
;MOLXYZ=mol,XYZUNEX,<icarb_bp86_xyz>,</icarb_bp86_xyz>

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;AMPLITUDES=mol,FREEU,<md_class_amp>,</md_class_amp>
;AMPLITUDES=mol,FREEU,<md_quant_c5>,</md_quant_c5>

GF=mol,AUTO,0.0486235

MINIMIZE=GEDINT+REGPRM,1-1,2-1,1000,2000

PRINT=GRAPHTERMS,mol

FUR=1-1,2-1

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B7	H18	1.2015	0.0800	-0.0163	73.3
B5	H16	1.2029	0.0800	-0.0163	74.2
B6	H17	1.2029	0.0800	-0.0163	74.2
B11	H22	1.2029	0.0800	-0.0163	74.2
B12	H23	1.2029	0.0800	-0.0163	74.2
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B10	H21	1.2043	0.0801	-0.0164	75.0
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C3	B11	1.6914	0.0672	-0.0130	56.9
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B6	B7	1.7724	0.0666	-0.0137	41.6
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B6	B8	1.7818	0.0680	-0.0127	47.9
B8	B12	1.7818	0.0680	-0.0127	47.9
B10	B11	1.7818	0.0680	-0.0127	47.9
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B9	B10	1.7953	0.0696	-0.0129	53.3
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B7	H14	2.3890	0.1180	-0.0185	9.4
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B11	H14	2.4412	0.1151	-0.0168	21.8
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C3	H22	2.4999	0.1225	-0.0181	21.5
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C3	H15	2.5054	0.1228	-0.0207	27.2
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B7	H17	2.5702	0.1274	-0.0165	-50.2
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B5	H21	2.6228	0.1262	-0.0151	-34.5
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B12	H18	2.6433	0.1227	-0.0165	-26.5
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B13	H19	2.6508	0.1258	-0.0172	-16.0
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B8	H17	2.6846	0.1224	-0.0152	-14.6

B8	H23	2.6846	0.1224	-0.0152	-14.6
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B10	H22	2.6846	0.1224	-0.0152	-14.6
B9	H16	2.6959	0.1216	-0.0160	-4.7
B9	H17	2.6959	0.1216	-0.0160	-4.7
B13	H22	2.6959	0.1216	-0.0160	-4.7
B13	H23	2.6959	0.1216	-0.0160	-4.7
B8	H18	2.7178	0.1186	-0.0135	-0.7
B10	H15	2.7178	0.1186	-0.0135	-0.7
C2	B9	2.7365	0.0696	-0.0200	17.6
C3	B13	2.7365	0.0696	-0.0200	17.6
C2	B11	2.7372	0.0716	-0.0207	26.6
C2	B12	2.7372	0.0716	-0.0207	26.6
C3	B5	2.7372	0.0716	-0.0207	26.6
C3	B6	2.7372	0.0716	-0.0207	26.6
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H1	H18	2.7382	0.1938	-0.0199	-132.5
H14	H15	2.7382	0.1938	-0.0199	-132.5
H14	H18	2.7382	0.1938	-0.0199	-132.5
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C2	B10	2.7433	0.0689	-0.0199	16.9
C3	B8	2.7433	0.0689	-0.0199	16.9
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H1	H17	2.8323	0.1906	-0.0154	-213.7
H14	H22	2.8323	0.1906	-0.0154	-213.7
H14	H23	2.8323	0.1906	-0.0154	-213.7
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B6	B12	2.8738	0.0723	-0.0210	19.8
B4	B9	2.8763	0.0729	-0.0205	19.4
B4	B13	2.8763	0.0729	-0.0205	19.4
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B7	B13	2.8763	0.0729	-0.0205	19.4
B4	B6	2.8807	0.0752	-0.0218	32.1
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B6	B13	2.8834	0.0737	-0.0202	20.1
B9	B11	2.8834	0.0737	-0.0202	20.1
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B8	B11	2.8910	0.0732	-0.0206	20.5
B10	B12	2.8910	0.0732	-0.0206	20.5
B4	B7	2.8947	0.0794	-0.0227	46.5
B8	B10	2.9094	0.0743	-0.0203	23.0
H16	H17	2.9724	0.2085	-0.0153	-372.2

H22	H23	2.9724	0.2085	-0.0153	-372.2
H15	H16	3.0209	0.2038	-0.0122	-412.5
H15	H22	3.0209	0.2038	-0.0122	-412.5
H17	H18	3.0209	0.2038	-0.0122	-412.5
H18	H23	3.0209	0.2038	-0.0122	-412.5
H16	H21	3.1419	0.2022	-0.0097	-512.2
H17	H19	3.1419	0.2022	-0.0097	-512.2
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H21	H22	3.1419	0.2022	-0.0097	-512.2
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H18	H19	3.1806	0.1974	-0.0054	-511.8
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C3	B9	3.2207	0.0714	-0.0233	2.6
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B6	I20	3.4292	0.1130	-0.0085	15.2
B11	I24	3.4292	0.1130	-0.0085	15.2
B12	I24	3.4292	0.1130	-0.0085	15.2
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B10	I20	3.4715	0.1146	-0.0149	32.8
B10	I24	3.4715	0.1146	-0.0149	32.8
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B13	I20	3.4905	0.1082	-0.0187	77.4
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H1	B12	3.6598	0.1090	-0.0269	30.4
B5	H14	3.6598	0.1090	-0.0269	30.4
B6	H14	3.6598	0.1090	-0.0269	30.4
H19	I20	3.6966	0.2173	-0.0133	-207.4
H19	I24	3.6966	0.2173	-0.0133	-207.4
I20	H21	3.6966	0.2173	-0.0133	-207.4
H21	I24	3.6966	0.2173	-0.0133	-207.4
H1	B8	3.7100	0.1061	-0.0253	20.1
H1	B10	3.7100	0.1061	-0.0253	20.1
B8	H14	3.7100	0.1061	-0.0253	20.1
B10	H14	3.7100	0.1061	-0.0253	20.1
H1	B9	3.7329	0.1046	-0.0251	35.8
B13	H14	3.7329	0.1046	-0.0251	35.8
H16	I20	3.7377	0.2098	-0.0006	-394.2
H17	I20	3.7377	0.2098	-0.0006	-394.2
H22	I24	3.7377	0.2098	-0.0006	-394.2
H23	I24	3.7377	0.2098	-0.0006	-394.2
C2	H22	3.7694	0.1150	-0.0256	21.2
C2	H23	3.7694	0.1150	-0.0256	21.2
C3	H16	3.7694	0.1150	-0.0256	21.2

C3	H17	3.7694	0.1150	-0.0256	21.2
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B7	H22	3.9000	0.1191	-0.0268	15.4
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B12	H17	3.9546	0.1143	-0.0247	9.6
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B6	H21	3.9708	0.1151	-0.0247	12.5
B11	H19	3.9708	0.1151	-0.0247	12.5
B12	H21	3.9708	0.1151	-0.0247	12.5
B8	H16	3.9819	0.1143	-0.0248	15.4
B8	H22	3.9819	0.1143	-0.0248	15.4
B10	H17	3.9819	0.1143	-0.0248	15.4
B10	H23	3.9819	0.1143	-0.0248	15.4
B8	H21	3.9958	0.1154	-0.0251	20.2
B10	H19	3.9958	0.1154	-0.0251	20.2
B9	H15	4.0037	0.1113	-0.0239	36.2
B9	H18	4.0037	0.1113	-0.0239	36.2
B13	H15	4.0037	0.1113	-0.0239	36.2
B13	H18	4.0037	0.1113	-0.0239	36.2
B9	H22	4.0134	0.1117	-0.0238	40.4
B9	H23	4.0134	0.1117	-0.0238	40.4
B13	H16	4.0134	0.1117	-0.0238	40.4
B13	H17	4.0134	0.1117	-0.0238	40.4
I20	I24	4.1883	0.2151	-0.0293	1882.7
H1	B13	4.3087	0.0996	-0.0298	51.3
B9	H14	4.3087	0.0996	-0.0298	51.3
H1	H22	4.5605	0.1559	-0.0303	-133.0
H1	H23	4.5605	0.1559	-0.0303	-133.0
H14	H16	4.5605	0.1559	-0.0303	-133.0
H14	H17	4.5605	0.1559	-0.0303	-133.0
B5	H23	4.5754	0.1059	-0.0296	61.9
B6	H22	4.5754	0.1059	-0.0296	61.9
B11	H17	4.5754	0.1059	-0.0296	61.9
B12	H16	4.5754	0.1059	-0.0296	61.9

B8	H15	4.5831	0.1062	-0.0301	59.4
B10	H18	4.5831	0.1062	-0.0301	59.4
B4	H19	4.6012	0.1056	-0.0288	64.8
B7	H21	4.6012	0.1056	-0.0288	64.8
H15	H18	4.6808	0.1723	-0.0374	-172.1
H1	H19	4.6986	0.1501	-0.0262	-140.3
H1	H21	4.6986	0.1501	-0.0262	-140.3
H14	H19	4.6986	0.1501	-0.0262	-140.3
H14	H21	4.6986	0.1501	-0.0262	-140.3
C2	I20	4.7169	0.0951	-0.0167	5.9
C3	I24	4.7169	0.0951	-0.0167	5.9
H15	H17	4.7999	0.1661	-0.0312	-203.4
H15	H23	4.7999	0.1661	-0.0312	-203.4
H16	H18	4.7999	0.1661	-0.0312	-203.4
H18	H22	4.7999	0.1661	-0.0312	-203.4
B4	I20	4.8442	0.1017	-0.0191	-12.5
B4	I24	4.8442	0.1017	-0.0191	-12.5
B7	I20	4.8442	0.1017	-0.0191	-12.5
B7	I24	4.8442	0.1017	-0.0191	-12.5
B5	I24	4.8781	0.0986	-0.0236	15.2
B6	I24	4.8781	0.0986	-0.0236	15.2
B11	I20	4.8781	0.0986	-0.0236	15.2
B12	I20	4.8781	0.0986	-0.0236	15.2
H16	H22	4.9384	0.1589	-0.0260	-219.5
H17	H23	4.9384	0.1589	-0.0260	-219.5
H16	H19	4.9701	0.1581	-0.0267	-190.9
H17	H21	4.9701	0.1581	-0.0267	-190.9
H19	H22	4.9701	0.1581	-0.0267	-190.9
H21	H23	4.9701	0.1581	-0.0267	-190.9
H19	H21	4.9892	0.1582	-0.0285	-168.2
C2	I24	5.3850	0.0802	-0.0243	28.7
C3	I20	5.3850	0.0802	-0.0243	28.7
H1	I20	5.5718	0.1421	-0.0173	-168.4
H14	I24	5.5718	0.1421	-0.0173	-168.4
H16	H23	5.7640	0.1308	-0.0335	109.8
H17	H22	5.7640	0.1308	-0.0335	109.8
H15	H19	5.7853	0.1303	-0.0335	115.2
H18	H21	5.7853	0.1303	-0.0335	115.2
H15	I20	5.8412	0.1531	-0.0178	-275.8
H15	I24	5.8412	0.1531	-0.0178	-275.8
H18	I20	5.8412	0.1531	-0.0178	-275.8
H18	I24	5.8412	0.1531	-0.0178	-275.8
H16	I24	5.8868	0.1487	-0.0248	-189.9
H17	I24	5.8868	0.1487	-0.0248	-189.9
I20	H22	5.8868	0.1487	-0.0248	-189.9
I20	H23	5.8868	0.1487	-0.0248	-189.9
H1	I24	6.4715	0.1065	-0.0289	75.8
H14	I20	6.4715	0.1065	-0.0289	75.8

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RENUM=1-1,2-14,3-2,4-3,5-4,6-7,7-5,8-6

RENUM=9-11,10-12,11-8,12-10,13-9,14-13,15-15,16-18

RENUM=17-16,18-17,19-22,20-23,21-19,22-21,23-20,24-24

H1	C3	1.0915	0.0459	-0.0051	23.0
H2	C4	1.0915	0.0459	-0.0051	23.0
B5	H15	1.2015	0.0364	-0.0045	1.7
B6	H16	1.2015	0.0364	-0.0045	1.7
B7	H17	1.2029	0.0522	-0.0065	72.7
B8	H18	1.2029	0.0522	-0.0065	72.7
B9	H19	1.2029	0.0522	-0.0065	72.7
B10	H20	1.2029	0.0522	-0.0065	72.7
B11	H21	1.2043	0.0637	-0.0087	45.4
B12	H22	1.2043	0.0637	-0.0087	45.4
C3	C4	1.6116	0.0369	-0.0030	10.9
C3	B7	1.6914	0.0470	-0.0068	22.4
C3	B8	1.6914	0.0470	-0.0068	22.4
C4	B9	1.6914	0.0470	-0.0068	22.4
C4	B10	1.6914	0.0470	-0.0068	22.4
C4	B5	1.7080	0.0466	-0.0059	28.1
C4	B6	1.7080	0.0466	-0.0059	28.1
C3	B5	1.7080	0.0466	-0.0059	28.1
C3	B6	1.7080	0.0466	-0.0059	28.1
B6	B11	1.7657	0.0397	-0.0084	12.8
B5	B12	1.7657	0.0397	-0.0084	12.8
B5	B7	1.7724	0.0462	-0.0056	12.0
B5	B9	1.7724	0.0462	-0.0056	12.0
B6	B8	1.7724	0.0462	-0.0056	12.0
B6	B10	1.7724	0.0462	-0.0056	12.0
B10	B14	1.7805	0.0469	-0.0078	24.1
B7	B13	1.7805	0.0469	-0.0078	24.1
B9	B14	1.7805	0.0469	-0.0078	24.1
B8	B13	1.7805	0.0469	-0.0078	24.1
B7	B8	1.7815	0.0464	-0.0061	11.0
B9	B10	1.7815	0.0464	-0.0061	11.0
B9	B12	1.7818	0.0488	-0.0067	22.0
B8	B11	1.7818	0.0488	-0.0067	22.0
B7	B12	1.7818	0.0488	-0.0067	22.0
B10	B11	1.7818	0.0488	-0.0067	22.0
B13	B14	1.7898	0.0431	-0.0161	2.3
B12	B13	1.7953	0.0497	-0.0089	41.9
B12	B14	1.7953	0.0497	-0.0089	41.9
B11	B14	1.7953	0.0497	-0.0089	41.9
B11	B13	1.7953	0.0497	-0.0089	41.9
B13	I23	2.1649	0.0565	-0.0212	49.6
B14	I24	2.1649	0.0565	-0.0212	49.6

H2	C3	2.3153	0.0634	-0.0068	28.1
H1	C4	2.3153	0.0634	-0.0068	28.1
H1	B5	2.3890	0.0657	-0.0094	47.0
H1	B6	2.3890	0.0657	-0.0094	47.0
H2	B5	2.3890	0.0657	-0.0094	47.0
H2	B6	2.3890	0.0657	-0.0094	47.0
H1	B7	2.4412	0.0684	-0.0084	38.4
H1	B8	2.4412	0.0684	-0.0084	38.4
H2	B9	2.4412	0.0684	-0.0084	38.4
H2	B10	2.4412	0.0684	-0.0084	38.4
C4	H20	2.4999	0.0790	-0.0077	46.9
C3	H17	2.4999	0.0790	-0.0077	46.9
C3	H18	2.4999	0.0790	-0.0077	46.9
C4	H19	2.4999	0.0790	-0.0077	46.9
C3	H16	2.5054	0.0775	-0.0066	8.2
C4	H15	2.5054	0.0775	-0.0066	8.2
C4	H16	2.5054	0.0775	-0.0066	8.2
C3	H15	2.5054	0.0775	-0.0066	8.2
B6	H20	2.5702	0.0900	-0.0046	23.1
B5	H17	2.5702	0.0900	-0.0046	23.1
B5	H19	2.5702	0.0900	-0.0046	23.1
B6	H18	2.5702	0.0900	-0.0046	23.1
H1	H2	2.5870	0.1221	-0.0056	-3.7
B6	H21	2.5939	0.0863	-0.0064	59.9
B5	H22	2.5939	0.0863	-0.0064	59.9
B7	H18	2.5966	0.0850	-0.0073	59.4
B10	H19	2.5966	0.0850	-0.0073	59.4
B9	H20	2.5966	0.0850	-0.0073	59.4
B8	H17	2.5966	0.0850	-0.0073	59.4
B9	H22	2.6228	0.0923	-0.0086	36.8
B8	H21	2.6228	0.0923	-0.0086	36.8
B10	H21	2.6228	0.0923	-0.0086	36.8
B7	H22	2.6228	0.0923	-0.0086	36.8
B9	H15	2.6433	0.0792	-0.0037	-3.4
B7	H15	2.6433	0.0792	-0.0037	-3.4
B8	H16	2.6433	0.0792	-0.0037	-3.4
B10	H16	2.6433	0.0792	-0.0037	-3.4
B13	H21	2.6508	0.0901	-0.0145	82.6
B14	H21	2.6508	0.0901	-0.0145	82.6
B14	H22	2.6508	0.0901	-0.0145	82.6
B13	H22	2.6508	0.0901	-0.0145	82.6
B11	H20	2.6846	0.0867	-0.0068	27.2
B11	H18	2.6846	0.0867	-0.0068	27.2
B12	H17	2.6846	0.0867	-0.0068	27.2
B12	H19	2.6846	0.0867	-0.0068	27.2
B14	H20	2.6959	0.0803	-0.0072	67.6
B13	H18	2.6959	0.0803	-0.0072	67.6
B13	H17	2.6959	0.0803	-0.0072	67.6

B14	H19	2.6959	0.0803	-0.0072	67.6
B11	H16	2.7178	0.0712	-0.0048	-15.9
B12	H15	2.7178	0.0712	-0.0048	-15.9
C4	B14	2.7365	0.0445	-0.0144	14.0
C3	B13	2.7365	0.0445	-0.0144	14.0
C4	B7	2.7372	0.0499	-0.0078	16.7
C4	B8	2.7372	0.0499	-0.0078	16.7
C3	B10	2.7372	0.0499	-0.0078	16.7
C3	B9	2.7372	0.0499	-0.0078	16.7
H2	H15	2.7382	0.1199	-0.0089	28.3
H2	H16	2.7382	0.1199	-0.0089	28.3
H1	H15	2.7382	0.1199	-0.0089	28.3
H1	H16	2.7382	0.1199	-0.0089	28.3
C3	B12	2.7433	0.0563	-0.0108	19.9
C3	B11	2.7433	0.0563	-0.0108	19.9
C4	B11	2.7433	0.0563	-0.0108	19.9
C4	B12	2.7433	0.0563	-0.0108	19.9
H2	H19	2.8323	0.1226	-0.0052	50.2
H2	H20	2.8323	0.1226	-0.0052	50.2
H1	H17	2.8323	0.1226	-0.0052	50.2
H1	H18	2.8323	0.1226	-0.0052	50.2
B7	B9	2.8738	0.0447	-0.0092	4.5
B8	B10	2.8738	0.0447	-0.0092	4.5
B6	B14	2.8763	0.0549	-0.0136	23.9
B5	B14	2.8763	0.0549	-0.0136	23.9
B5	B13	2.8763	0.0549	-0.0136	23.9
B6	B13	2.8763	0.0549	-0.0136	23.9
B6	B9	2.8807	0.0494	-0.0096	3.8
B5	B8	2.8807	0.0494	-0.0096	3.8
B6	B7	2.8807	0.0494	-0.0096	3.8
B5	B10	2.8807	0.0494	-0.0096	3.8
B7	B14	2.8834	0.0541	-0.0147	10.4
B8	B14	2.8834	0.0541	-0.0147	10.4
B9	B13	2.8834	0.0541	-0.0147	10.4
B10	B13	2.8834	0.0541	-0.0147	10.4
B8	B12	2.8910	0.0569	-0.0096	-4.6
B7	B11	2.8910	0.0569	-0.0096	-4.6
B10	B12	2.8910	0.0569	-0.0096	-4.6
B9	B11	2.8910	0.0569	-0.0096	-4.6
B5	B6	2.8947	0.0327	-0.0116	2.7
B11	B12	2.9094	0.0397	-0.0101	3.1
H17	H18	2.9724	0.1530	-0.0041	88.9
H19	H20	2.9724	0.1530	-0.0041	88.9
H16	H18	3.0209	0.1415	-0.0000	-69.7
H16	H20	3.0209	0.1415	-0.0000	-69.7
H15	H17	3.0209	0.1415	-0.0000	-69.7
H15	H19	3.0209	0.1415	-0.0000	-69.7
H18	H21	3.1419	0.1395	-0.0051	-11.0

H17	H22	3.1419	0.1395	-0.0051	-11.0
H19	H22	3.1419	0.1395	-0.0051	-11.0
H20	H21	3.1419	0.1395	-0.0051	-11.0
H15	H22	3.1806	0.1190	0.0009	45.5
H16	H21	3.1806	0.1190	0.0009	45.5
C3	B14	3.2207	0.0484	-0.0159	-3.1
C4	B13	3.2207	0.0484	-0.0159	-3.1
B7	B10	3.3812	0.0556	-0.0104	-8.4
B8	B9	3.3812	0.0556	-0.0104	-8.4
B5	B11	3.3970	0.0533	-0.0125	2.7
B6	B12	3.3970	0.0533	-0.0125	2.7
B9	I24	3.4292	0.1209	0.0067	260.8
B8	I23	3.4292	0.1209	0.0067	260.8
B7	I23	3.4292	0.1209	0.0067	260.8
B10	I24	3.4292	0.1209	0.0067	260.8
B12	I24	3.4715	0.1633	-0.0187	384.2
B11	I23	3.4715	0.1633	-0.0187	384.2
B11	I24	3.4715	0.1633	-0.0187	384.2
B12	I23	3.4715	0.1633	-0.0187	384.2
B14	I23	3.4905	0.1509	-0.0417	-338.4
B13	I24	3.4905	0.1509	-0.0417	-338.4
H1	B9	3.6598	0.0691	-0.0119	26.7
H1	B10	3.6598	0.0691	-0.0119	26.7
H2	B7	3.6598	0.0691	-0.0119	26.7
H2	B8	3.6598	0.0691	-0.0119	26.7
H21	I23	3.6966	0.2707	-0.0182	525.7
H21	I24	3.6966	0.2707	-0.0182	525.7
H22	I23	3.6966	0.2707	-0.0182	525.7
H22	I24	3.6966	0.2707	-0.0182	525.7
H2	B11	3.7100	0.0680	-0.0142	23.0
H2	B12	3.7100	0.0680	-0.0142	23.0
H1	B11	3.7100	0.0680	-0.0142	23.0
H1	B12	3.7100	0.0680	-0.0142	23.0
H1	B13	3.7329	0.0647	-0.0158	34.6
H2	B14	3.7329	0.0647	-0.0158	34.6
H18	I23	3.7377	0.2149	0.0293	1058.1
H19	I24	3.7377	0.2149	0.0293	1058.1
H17	I23	3.7377	0.2149	0.0293	1058.1
H20	I24	3.7377	0.2149	0.0293	1058.1
C4	H18	3.7694	0.0772	-0.0080	37.1
C3	H19	3.7694	0.0772	-0.0080	37.1
C3	H20	3.7694	0.0772	-0.0080	37.1
C4	H17	3.7694	0.0772	-0.0080	37.1
C3	H22	3.8278	0.0868	-0.0124	67.1
C4	H21	3.8278	0.0868	-0.0124	67.1
C4	H22	3.8278	0.0868	-0.0124	67.1
C3	H21	3.8278	0.0868	-0.0124	67.1
B5	H16	3.8721	0.0639	-0.0123	-3.5

B6	H15	3.8721	0.0639	-0.0123	-3.5
B5	H20	3.9000	0.0779	-0.0106	26.5
B6	H19	3.9000	0.0779	-0.0106	26.5
B5	H18	3.9000	0.0779	-0.0106	26.5
B6	H17	3.9000	0.0779	-0.0106	26.5
B10	H15	3.9149	0.0717	-0.0089	-13.6
B9	H16	3.9149	0.0717	-0.0089	-13.6
B8	H15	3.9149	0.0717	-0.0089	-13.6
B7	H16	3.9149	0.0717	-0.0089	-13.6
B8	H20	3.9546	0.0777	-0.0096	43.3
B10	H18	3.9546	0.0777	-0.0096	43.3
B7	H19	3.9546	0.0777	-0.0096	43.3
B9	H17	3.9546	0.0777	-0.0096	43.3
B10	H22	3.9708	0.0866	-0.0146	57.0
B8	H22	3.9708	0.0866	-0.0146	57.0
B7	H21	3.9708	0.0866	-0.0146	57.0
B9	H21	3.9708	0.0866	-0.0146	57.0
B11	H19	3.9819	0.0813	-0.0110	61.7
B12	H18	3.9819	0.0813	-0.0110	61.7
B11	H17	3.9819	0.0813	-0.0110	61.7
B12	H20	3.9819	0.0813	-0.0110	61.7
B11	H22	3.9958	0.0727	-0.0166	48.6
B12	H21	3.9958	0.0727	-0.0166	48.6
B14	H15	4.0037	0.0722	-0.0107	19.1
B14	H16	4.0037	0.0722	-0.0107	19.1
B13	H15	4.0037	0.0722	-0.0107	19.1
B13	H16	4.0037	0.0722	-0.0107	19.1
B14	H17	4.0134	0.0788	-0.0158	65.9
B14	H18	4.0134	0.0788	-0.0158	65.9
B13	H19	4.0134	0.0788	-0.0158	65.9
B13	H20	4.0134	0.0788	-0.0158	65.9
I23	I24	4.1883	0.3383	-0.0898	-7612.4
H1	B14	4.3087	0.0645	-0.0196	13.7
H2	B13	4.3087	0.0645	-0.0196	13.7
H1	H20	4.5605	0.0972	-0.0114	51.6
H2	H17	4.5605	0.0972	-0.0114	51.6
H2	H18	4.5605	0.0972	-0.0114	51.6
H1	H19	4.5605	0.0972	-0.0114	51.6
B10	H17	4.5754	0.0736	-0.0117	55.6
B9	H18	4.5754	0.0736	-0.0117	55.6
B7	H20	4.5754	0.0736	-0.0117	55.6
B8	H19	4.5754	0.0736	-0.0117	55.6
B11	H15	4.5831	0.0651	-0.0113	-0.1
B12	H16	4.5831	0.0651	-0.0113	-0.1
B6	H22	4.6012	0.0791	-0.0167	44.6
B5	H21	4.6012	0.0791	-0.0167	44.6
H15	H16	4.6808	0.1095	-0.0130	-93.3
H1	H21	4.6986	0.1016	-0.0137	61.1

H1	H22	4.6986	0.1016	-0.0137	61.1
H2	H21	4.6986	0.1016	-0.0137	61.1
H2	H22	4.6986	0.1016	-0.0137	61.1
C4	I24	4.7169	0.0784	0.0021	40.7
C3	I23	4.7169	0.0784	0.0021	40.7
H16	H17	4.7999	0.0993	-0.0102	-7.0
H15	H20	4.7999	0.0993	-0.0102	-7.0
H16	H19	4.7999	0.0993	-0.0102	-7.0
H15	H18	4.7999	0.0993	-0.0102	-7.0
B6	I23	4.8442	0.1201	-0.0063	23.3
B6	I24	4.8442	0.1201	-0.0063	23.3
B5	I23	4.8442	0.1201	-0.0063	23.3
B5	I24	4.8442	0.1201	-0.0063	23.3
B9	I23	4.8781	0.1332	-0.0281	43.2
B8	I24	4.8781	0.1332	-0.0281	43.2
B10	I23	4.8781	0.1332	-0.0281	43.2
B7	I24	4.8781	0.1332	-0.0281	43.2
H17	H19	4.9384	0.1090	-0.0092	-7.3
H18	H20	4.9384	0.1090	-0.0092	-7.3
H19	H21	4.9701	0.1110	-0.0154	53.2
H20	H22	4.9701	0.1110	-0.0154	53.2
H17	H21	4.9701	0.1110	-0.0154	53.2
H18	H22	4.9701	0.1110	-0.0154	53.2
H21	H22	4.9892	0.1034	-0.0235	-36.0
C4	I23	5.3850	0.0771	-0.0141	45.5
C3	I24	5.3850	0.0771	-0.0141	45.5
H2	I24	5.5718	0.1165	0.0120	55.6
H1	I23	5.5718	0.1165	0.0120	55.6
H18	H19	5.7640	0.0883	-0.0127	21.7
H17	H20	5.7640	0.0883	-0.0127	21.7
H15	H21	5.7853	0.0887	-0.0156	11.2
H16	H22	5.7853	0.0887	-0.0156	11.2
H15	I23	5.8412	0.1613	0.0052	-345.1
H15	I24	5.8412	0.1613	0.0052	-345.1
H16	I23	5.8412	0.1613	0.0052	-345.1
H16	I24	5.8412	0.1613	0.0052	-345.1
H20	I23	5.8868	0.1723	-0.0313	-217.6
H18	I24	5.8868	0.1723	-0.0313	-217.6
H17	I24	5.8868	0.1723	-0.0313	-217.6
H19	I23	5.8868	0.1723	-0.0313	-217.6
H1	I24	6.4715	0.0866	-0.0144	44.0
H2	I23	6.4715	0.0866	-0.0144	44.0

</md_class_amp>

<md_quant_c5>

RENUM=1-1,2-14,3-2,4-3,5-4,6-7,7-5,8-6

RENUM=9-11,10-12,11-8,12-10,13-9,14-13,15-15,16-18

RENUM=17-16,18-17,19-22,20-23,21-19,22-21,23-20,24-24

H1	C3	1.0915	0.0634	-0.0383	215.8
H2	C4	1.0915	0.0634	-0.0383	215.8
B5	H15	1.2015	0.0618	-0.0494	255.0
B6	H16	1.2015	0.0618	-0.0494	255.0
B7	H17	1.2029	0.0740	0.0303	-217.3
B8	H18	1.2029	0.0740	0.0303	-217.3
B9	H19	1.2029	0.0740	0.0303	-217.3
B10	H20	1.2029	0.0740	0.0303	-217.3
B11	H21	1.2043	0.0780	-0.0246	199.3
B12	H22	1.2043	0.0780	-0.0246	199.3
C3	C4	1.6116	0.0604	-0.0105	54.7
C3	B7	1.6914	0.0666	-0.0163	111.7
C3	B8	1.6914	0.0666	-0.0163	111.7
C4	B9	1.6914	0.0666	-0.0163	111.7
C4	B10	1.6914	0.0666	-0.0163	111.7
C4	B5	1.7080	0.0696	-0.0044	0.1
C4	B6	1.7080	0.0696	-0.0044	0.1
C3	B5	1.7080	0.0696	-0.0044	0.1
C3	B6	1.7080	0.0696	-0.0044	0.1
B6	B11	1.7657	0.0668	-0.0183	95.8
B5	B12	1.7657	0.0668	-0.0183	95.8
B5	B7	1.7724	0.0666	-0.0154	105.4
B5	B9	1.7724	0.0666	-0.0154	105.4
B6	B8	1.7724	0.0666	-0.0154	105.4
B6	B10	1.7724	0.0666	-0.0154	105.4
B10	B14	1.7805	0.0718	-0.0100	41.6
B7	B13	1.7805	0.0718	-0.0100	41.6
B9	B14	1.7805	0.0718	-0.0100	41.6
B8	B13	1.7805	0.0718	-0.0100	41.6
B7	B8	1.7815	0.0669	-0.0106	55.8
B9	B10	1.7815	0.0669	-0.0106	55.8
B9	B12	1.7818	0.0691	-0.0142	97.6
B8	B11	1.7818	0.0691	-0.0142	97.6
B7	B12	1.7818	0.0691	-0.0142	97.6
B10	B11	1.7818	0.0691	-0.0142	97.6
B13	B14	1.7898	0.0729	-0.0164	23.4
B12	B13	1.7953	0.0711	-0.0225	191.2
B12	B14	1.7953	0.0711	-0.0225	191.2
B11	B14	1.7953	0.0711	-0.0225	191.2
B11	B13	1.7953	0.0711	-0.0225	191.2
B13	I23	2.1649	0.0755	-0.0383	435.5
B14	I24	2.1649	0.0755	-0.0383	435.5
H2	C3	2.3153	0.0989	-0.0105	72.7
H1	C4	2.3153	0.0989	-0.0105	72.7
H1	B5	2.3890	0.1035	-0.0121	70.0
H1	B6	2.3890	0.1035	-0.0121	70.0
H2	B5	2.3890	0.1035	-0.0121	70.0
H2	B6	2.3890	0.1035	-0.0121	70.0

H1	B7	2.4412	0.1023	-0.0129	93.2
H1	B8	2.4412	0.1023	-0.0129	93.2
H2	B9	2.4412	0.1023	-0.0129	93.2
H2	B10	2.4412	0.1023	-0.0129	93.2
C4	H20	2.4999	0.1118	-0.0118	124.7
C3	H17	2.4999	0.1118	-0.0118	124.7
C3	H18	2.4999	0.1118	-0.0118	124.7
C4	H19	2.4999	0.1118	-0.0118	124.7
C3	H16	2.5054	0.1254	-0.0059	65.2
C4	H15	2.5054	0.1254	-0.0059	65.2
C4	H16	2.5054	0.1254	-0.0059	65.2
C3	H15	2.5054	0.1254	-0.0059	65.2
B6	H20	2.5702	0.1200	-0.0055	86.8
B5	H17	2.5702	0.1200	-0.0055	86.8
B5	H19	2.5702	0.1200	-0.0055	86.8
B6	H18	2.5702	0.1200	-0.0055	86.8
H1	H2	2.5870	0.1677	-0.0056	235.4
B6	H21	2.5939	0.1080	-0.0079	75.0
B5	H22	2.5939	0.1080	-0.0079	75.0
B7	H18	2.5966	0.1179	-0.0041	-13.9
B10	H19	2.5966	0.1179	-0.0041	-13.9
B9	H20	2.5966	0.1179	-0.0041	-13.9
B8	H17	2.5966	0.1179	-0.0041	-13.9
B9	H22	2.6228	0.1106	-0.0093	62.4
B8	H21	2.6228	0.1106	-0.0093	62.4
B10	H21	2.6228	0.1106	-0.0093	62.4
B7	H22	2.6228	0.1106	-0.0093	62.4
B9	H15	2.6433	0.1268	-0.0001	1.3
B7	H15	2.6433	0.1268	-0.0001	1.3
B8	H16	2.6433	0.1268	-0.0001	1.3
B10	H16	2.6433	0.1268	-0.0001	1.3
B13	H21	2.6508	0.1100	-0.0164	96.1
B14	H21	2.6508	0.1100	-0.0164	96.1
B14	H22	2.6508	0.1100	-0.0164	96.1
B13	H22	2.6508	0.1100	-0.0164	96.1
B11	H20	2.6846	0.1162	-0.0024	-50.2
B11	H18	2.6846	0.1162	-0.0024	-50.2
B12	H17	2.6846	0.1162	-0.0024	-50.2
B12	H19	2.6846	0.1162	-0.0024	-50.2
B14	H20	2.6959	0.1126	-0.0068	36.8
B13	H18	2.6959	0.1126	-0.0068	36.8
B13	H17	2.6959	0.1126	-0.0068	36.8
B14	H19	2.6959	0.1126	-0.0068	36.8
B11	H16	2.7178	0.1198	0.0017	-53.8
B12	H15	2.7178	0.1198	0.0017	-53.8
C4	B14	2.7365	0.0727	-0.0162	34.2
C3	B13	2.7365	0.0727	-0.0162	34.2
C4	B7	2.7372	0.0698	-0.0122	62.1

C4	B8	2.7372	0.0698	-0.0122	62.1
C3	B10	2.7372	0.0698	-0.0122	62.1
C3	B9	2.7372	0.0698	-0.0122	62.1
H2	H15	2.7382	0.1893	-0.0101	488.0
H2	H16	2.7382	0.1893	-0.0101	488.0
H1	H15	2.7382	0.1893	-0.0101	488.0
H1	H16	2.7382	0.1893	-0.0101	488.0
C3	B12	2.7433	0.0701	-0.0148	77.5
C3	B11	2.7433	0.0701	-0.0148	77.5
C4	B11	2.7433	0.0701	-0.0148	77.5
C4	B12	2.7433	0.0701	-0.0148	77.5
H2	H19	2.8323	0.1767	-0.0082	436.7
H2	H20	2.8323	0.1767	-0.0082	436.7
H1	H17	2.8323	0.1767	-0.0082	436.7
H1	H18	2.8323	0.1767	-0.0082	436.7
B7	B9	2.8738	0.0663	-0.0194	102.6
B8	B10	2.8738	0.0663	-0.0194	102.6
B6	B14	2.8763	0.0774	-0.0198	117.3
B5	B14	2.8763	0.0774	-0.0198	117.3
B5	B13	2.8763	0.0774	-0.0198	117.3
B6	B13	2.8763	0.0774	-0.0198	117.3
B6	B9	2.8807	0.0731	-0.0196	135.5
B5	B8	2.8807	0.0731	-0.0196	135.5
B6	B7	2.8807	0.0731	-0.0196	135.5
B5	B10	2.8807	0.0731	-0.0196	135.5
B7	B14	2.8834	0.0788	-0.0196	98.3
B8	B14	2.8834	0.0788	-0.0196	98.3
B9	B13	2.8834	0.0788	-0.0196	98.3
B10	B13	2.8834	0.0788	-0.0196	98.3
B8	B12	2.8910	0.0741	-0.0095	10.1
B7	B11	2.8910	0.0741	-0.0095	10.1
B10	B12	2.8910	0.0741	-0.0095	10.1
B9	B11	2.8910	0.0741	-0.0095	10.1
B5	B6	2.8947	0.0633	-0.0318	160.7
B11	B12	2.9094	0.0647	-0.0143	38.5
H17	H18	2.9724	0.1997	0.0023	-86.4
H19	H20	2.9724	0.1997	0.0023	-86.4
H16	H18	3.0209	0.1985	0.0103	-292.4
H16	H20	3.0209	0.1985	0.0103	-292.4
H15	H17	3.0209	0.1985	0.0103	-292.4
H15	H19	3.0209	0.1985	0.0103	-292.4
H18	H21	3.1419	0.1790	0.0011	-152.1
H17	H22	3.1419	0.1790	0.0011	-152.1
H19	H22	3.1419	0.1790	0.0011	-152.1
H20	H21	3.1419	0.1790	0.0011	-152.1
H15	H22	3.1806	0.1784	0.0141	-366.7
H16	H21	3.1806	0.1784	0.0141	-366.7
C3	B14	3.2207	0.0783	-0.0026	-162.5

C4	B13	3.2207	0.0783	-0.0026	-162.5
B7	B10	3.3812	0.0727	-0.0119	31.4
B8	B9	3.3812	0.0727	-0.0119	31.4
B5	B11	3.3970	0.0725	-0.0167	69.7
B6	B12	3.3970	0.0725	-0.0167	69.7
B9	I24	3.4292	0.1417	-0.0028	1442.9
B8	I23	3.4292	0.1417	-0.0028	1442.9
B7	I23	3.4292	0.1417	-0.0028	1442.9
B10	I24	3.4292	0.1417	-0.0028	1442.9
B12	I24	3.4715	0.1565	-0.0177	1193.9
B11	I23	3.4715	0.1565	-0.0177	1193.9
B11	I24	3.4715	0.1565	-0.0177	1193.9
B12	I23	3.4715	0.1565	-0.0177	1193.9
B14	I23	3.4905	0.1622	-0.0427	671.2
B13	I24	3.4905	0.1622	-0.0427	671.2
H1	B9	3.6598	0.0983	-0.0179	99.9
H1	B10	3.6598	0.0983	-0.0179	99.9
H2	B7	3.6598	0.0983	-0.0179	99.9
H2	B8	3.6598	0.0983	-0.0179	99.9
H21	I23	3.6966	0.2881	-0.0229	6844.2
H21	I24	3.6966	0.2881	-0.0229	6844.2
H22	I23	3.6966	0.2881	-0.0229	6844.2
H22	I24	3.6966	0.2881	-0.0229	6844.2
H2	B11	3.7100	0.0979	-0.0150	28.0
H2	B12	3.7100	0.0979	-0.0150	28.0
H1	B11	3.7100	0.0979	-0.0150	28.0
H1	B12	3.7100	0.0979	-0.0150	28.0
H1	B13	3.7329	0.0951	-0.0169	28.5
H2	B14	3.7329	0.0951	-0.0169	28.5
H18	I23	3.7377	0.2484	0.0297	1311.6
H19	I24	3.7377	0.2484	0.0297	1311.6
H17	I23	3.7377	0.2484	0.0297	1311.6
H20	I24	3.7377	0.2484	0.0297	1311.6
C4	H18	3.7694	0.1074	-0.0107	72.4
C3	H19	3.7694	0.1074	-0.0107	72.4
C3	H20	3.7694	0.1074	-0.0107	72.4
C4	H17	3.7694	0.1074	-0.0107	72.4
C3	H22	3.8278	0.1019	-0.0154	98.6
C4	H21	3.8278	0.1019	-0.0154	98.6
C4	H22	3.8278	0.1019	-0.0154	98.6
C3	H21	3.8278	0.1019	-0.0154	98.6
B5	H16	3.8721	0.1132	-0.0178	111.6
B6	H15	3.8721	0.1132	-0.0178	111.6
B5	H20	3.9000	0.1089	-0.0098	13.4
B6	H19	3.9000	0.1089	-0.0098	13.4
B5	H18	3.9000	0.1089	-0.0098	13.4
B6	H17	3.9000	0.1089	-0.0098	13.4
B10	H15	3.9149	0.1193	-0.0082	28.6

B9	H16	3.9149	0.1193	-0.0082	28.6
B8	H15	3.9149	0.1193	-0.0082	28.6
B7	H16	3.9149	0.1193	-0.0082	28.6
B8	H20	3.9546	0.1079	-0.0068	-24.9
B10	H18	3.9546	0.1079	-0.0068	-24.9
B7	H19	3.9546	0.1079	-0.0068	-24.9
B9	H17	3.9546	0.1079	-0.0068	-24.9
B10	H22	3.9708	0.1021	-0.0175	95.9
B8	H22	3.9708	0.1021	-0.0175	95.9
B7	H21	3.9708	0.1021	-0.0175	95.9
B9	H21	3.9708	0.1021	-0.0175	95.9
B11	H19	3.9819	0.1107	-0.0009	-178.8
B12	H18	3.9819	0.1107	-0.0009	-178.8
B11	H17	3.9819	0.1107	-0.0009	-178.8
B12	H20	3.9819	0.1107	-0.0009	-178.8
B11	H22	3.9958	0.0935	-0.0207	78.5
B12	H21	3.9958	0.0935	-0.0207	78.5
B14	H15	4.0037	0.1185	-0.0146	106.8
B14	H16	4.0037	0.1185	-0.0146	106.8
B13	H15	4.0037	0.1185	-0.0146	106.8
B13	H16	4.0037	0.1185	-0.0146	106.8
B14	H17	4.0134	0.1077	-0.0147	3.9
B14	H18	4.0134	0.1077	-0.0147	3.9
B13	H19	4.0134	0.1077	-0.0147	3.9
B13	H20	4.0134	0.1077	-0.0147	3.9
I23	I24	4.1883	0.2081	-0.0540	3488.7
H1	B14	4.3087	0.0924	-0.0213	32.9
H2	B13	4.3087	0.0924	-0.0213	32.9
H1	H20	4.5605	0.1429	-0.0104	36.9
H2	H17	4.5605	0.1429	-0.0104	36.9
H2	H18	4.5605	0.1429	-0.0104	36.9
H1	H19	4.5605	0.1429	-0.0104	36.9
B10	H17	4.5754	0.1032	-0.0095	-17.1
B9	H18	4.5754	0.1032	-0.0095	-17.1
B7	H20	4.5754	0.1032	-0.0095	-17.1
B8	H19	4.5754	0.1032	-0.0095	-17.1
B11	H15	4.5831	0.1107	-0.0190	132.8
B12	H16	4.5831	0.1107	-0.0190	132.8
B6	H22	4.6012	0.0951	-0.0198	77.7
B5	H21	4.6012	0.0951	-0.0198	77.7
H15	H16	4.6808	0.1778	-0.0062	-114.6
H1	H21	4.6986	0.1354	-0.0175	161.0
H1	H22	4.6986	0.1354	-0.0175	161.0
H2	H21	4.6986	0.1354	-0.0175	161.0
H2	H22	4.6986	0.1354	-0.0175	161.0
C4	I24	4.7169	0.0987	-0.0047	327.3
C3	I23	4.7169	0.0987	-0.0047	327.3
H16	H17	4.7999	0.1552	-0.0078	17.4

H15	H20	4.7999	0.1552	-0.0078	17.4
H16	H19	4.7999	0.1552	-0.0078	17.4
H15	H18	4.7999	0.1552	-0.0078	17.4
B6	I23	4.8442	0.1368	-0.0074	278.7
B6	I24	4.8442	0.1368	-0.0074	278.7
B5	I23	4.8442	0.1368	-0.0074	278.7
B5	I24	4.8442	0.1368	-0.0074	278.7
B9	I23	4.8781	0.1356	-0.0288	467.5
B8	I24	4.8781	0.1356	-0.0288	467.5
B10	I23	4.8781	0.1356	-0.0288	467.5
B7	I24	4.8781	0.1356	-0.0288	467.5
H17	H19	4.9384	0.1456	-0.0102	97.2
H18	H20	4.9384	0.1456	-0.0102	97.2
H19	H21	4.9701	0.1435	-0.0163	94.5
H20	H22	4.9701	0.1435	-0.0163	94.5
H17	H21	4.9701	0.1435	-0.0163	94.5
H18	H22	4.9701	0.1435	-0.0163	94.5
H21	H22	4.9892	0.1343	-0.0253	103.4
C4	I23	5.3850	0.0884	-0.0188	257.9
C3	I24	5.3850	0.0884	-0.0188	257.9
H2	I24	5.5718	0.1331	0.0093	219.7
H1	I23	5.5718	0.1331	0.0093	219.7
H18	H19	5.7640	0.1279	-0.0139	57.7
H17	H20	5.7640	0.1279	-0.0139	57.7
H15	H21	5.7853	0.1259	-0.0196	116.3
H16	H22	5.7853	0.1259	-0.0196	116.3
H15	I23	5.8412	0.2013	0.0144	-965.4
H15	I24	5.8412	0.2013	0.0144	-965.4
H16	I23	5.8412	0.2013	0.0144	-965.4
H16	I24	5.8412	0.2013	0.0144	-965.4
H20	I23	5.8868	0.1726	-0.0314	203.1
H18	I24	5.8868	0.1726	-0.0314	203.1
H17	I24	5.8868	0.1726	-0.0314	203.1
H19	I23	5.8868	0.1726	-0.0314	203.1
H1	I24	6.4715	0.1027	-0.0202	157.6
H2	I23	6.4715	0.1027	-0.0202	157.6

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2.60000000	-0.20970691
2.80000000	-0.21632349
3.00000000	-0.28228814
3.20000000	-0.37502978

3.40000000	-0.37542549
3.60000000	-0.21709592
3.80000000	0.07676726
4.00000000	0.35776994
4.20000000	0.49896728
4.40000000	0.45522378
4.60000000	0.28343342
4.80000000	0.10660670
5.00000000	0.01849161
5.20000000	0.03828454
5.40000000	0.07838255
5.60000000	0.05310510
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6.00000000	-0.26533469
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6.60000000	-0.24596942
6.80000000	-0.09076946
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7.40000000	0.16949974
7.60000000	0.25145341
7.80000000	0.32598446
8.00000000	0.31862609
8.20000000	0.20280038
8.40000000	0.00643804
8.60000000	-0.15990305
8.80000000	-0.21952770
9.00000000	-0.13395457
9.20000000	0.02017222
9.40000000	0.12349501
9.60000000	0.09738794
9.80000000	-0.04084614
10.00000000	-0.21563866
10.20000000	-0.32162352
10.40000000	-0.29844277
10.60000000	-0.18233291
10.80000000	-0.03314299
11.00000000	0.08487055
11.20000000	0.15990965
11.40000000	0.21968701
11.60000000	0.26352947
11.80000000	0.25698305
12.00000000	0.19656205
12.20000000	0.08709908
12.40000000	-0.02325200
12.60000000	-0.09484682
12.80000000	-0.11477113

13.00000000	-0.09996873
13.20000000	-0.07824956
13.40000000	-0.07837553
13.60000000	-0.10582993
13.80000000	-0.11268776
14.00000000	-0.10743608
14.20000000	-0.06171436
14.40000000	0.00146888
14.60000000	0.04677503
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15.00000000	0.09737753
15.20000000	0.11486153
15.40000000	0.11567302
15.60000000	0.10425444
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16.00000000	0.04392590
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6.20000000	-0.30680811
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8.00000000	0.24508280
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9.00000000	-0.10480453
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10.00000000	-0.16216839
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11.00000000	0.06547138
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11.60000000	0.20830614
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12.00000000	0.16056129
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13.60000000	-0.07915612
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14.00000000	-0.07951977
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14.60000000	0.03091434
14.80000000	0.06420981
15.00000000	0.08007944
15.20000000	0.09518599
15.40000000	0.09239892
15.60000000	0.08657044
15.80000000	0.05757547
16.00000000	0.02043737
16.20000000	-0.01452627
16.40000000	-0.05146118
16.60000000	-0.07966643
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17.00000000	-0.09244021
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17.80000000	0.01774610
18.00000000	0.03462456
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18.80000000	0.05933246
19.00000000	0.03337390
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19.40000000	0.00726027
19.60000000	-0.01627260
19.80000000	-0.02543111
20.00000000	-0.02878446
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20.40000000	-0.04181390
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20.80000000	-0.04416560
21.00000000	-0.03248962

21.20000000	-0.02186486
21.40000000	-0.00233394
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21.80000000	0.03814150
22.00000000	0.04274982
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22.40000000	0.05495689
22.60000000	0.02824633
22.80000000	0.02089072
23.00000000	0.00801496
23.20000000	-0.01432968
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23.60000000	-0.03034145
23.80000000	-0.02538729
24.00000000	-0.03720849
24.20000000	-0.02559133
24.40000000	-0.01892939
24.60000000	-0.01964235
24.80000000	-0.00187417
25.00000000	0.00149377
25.20000000	0.01196572
25.40000000	0.02470696
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26.00000000	0.01834421
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26.40000000	0.00260064
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27.00000000	-0.02887604
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27.40000000	-0.03707871
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27.80000000	-0.00260304
28.00000000	-0.02381533
28.20000000	0.02541713
28.40000000	0.01359314
28.60000000	0.01748108
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29.00000000	0.01479399
29.20000000	0.01036958
29.40000000	-0.00297139
29.60000000	0.01244592
29.80000000	-0.01066851
30.00000000	-0.01804497
30.20000000	-0.00818978
30.40000000	-0.01941423
30.60000000	0.01408375

30.80000000	-0.01287765
31.00000000	-0.00014054
31.20000000	-0.00266410
31.40000000	-0.02469729
31.60000000	0.04821582
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<icarb_mp2_xyz>

H	1.287579	0.000000	4.203739
C	0.811135	0.000000	3.234897
C	-0.811135	0.000000	3.234897
B	0.000000	1.454956	2.820646
B	1.438781	0.894285	1.941703
B	1.438781	-0.894285	1.941703
B	0.000000	-1.454956	2.820646
B	0.000000	-1.455265	1.054483
B	0.892769	0.000000	0.504310
B	0.000000	1.455265	1.054483
B	-1.438781	0.894285	1.941703
B	-1.438781	-0.894285	1.941703
B	-0.892769	0.000000	0.504310
H	-1.287579	0.000000	4.203739
H	0.000000	2.327729	3.612051
H	2.453953	1.474069	2.098171
H	2.453953	-1.474069	2.098171
H	0.000000	-2.327729	3.612051
H	0.000000	-2.470014	0.450560
I	2.080743	0.000000	-1.287892
H	0.000000	2.470014	0.450560
H	-2.453953	1.474069	2.098171
H	-2.453953	-1.474069	2.098171
I	-2.080743	0.000000	-1.287892

</icarb_mp2_xyz>

<icarb_b3lyp_xyz>

H	1.290605	0.000000	4.203131
C	0.811733	0.000000	3.238382
C	-0.811733	0.000000	3.238382
B	0.000000	1.451844	2.820067
B	1.436049	0.892041	1.944410
B	1.436049	-0.892041	1.944410
B	0.000000	-1.451844	2.820067
B	0.000000	-1.454099	1.059665
B	0.894221	0.000000	0.506937
B	0.000000	1.454099	1.059665
B	-1.436049	0.892041	1.944410
B	-1.436049	-0.892041	1.944410

B	-0.894221	0.000000	0.506937
H	-1.290605	0.000000	4.203131
H	0.000000	2.331422	3.599734
H	2.446664	1.474999	2.095377
H	2.446664	-1.474999	2.095377
H	0.000000	-2.331422	3.599734
H	0.000000	-2.469183	0.462926
I	2.122762	0.000000	-1.297874
H	0.000000	2.469183	0.462926
H	-2.446664	1.474999	2.095377
H	-2.446664	-1.474999	2.095377
I	-2.122762	0.000000	-1.297874

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<icarb_bp86_xyz>

H	1.299814	4.176527	-0.000001
C	0.817654	3.202984	0.000000
C	-0.818576	3.202745	0.000000
B	-0.000397	2.781112	-1.455701
B	1.441413	1.900021	-0.895269
B	1.441412	1.900020	0.895269
B	-0.000397	2.781113	1.455702
B	-0.000143	1.013067	1.457148
B	0.896827	0.458704	0.000000
B	-0.000143	1.013068	-1.457149
B	-1.441955	1.899604	-0.895270
B	-1.441954	1.899603	0.895270
B	-0.896952	0.458448	0.000000
H	-1.301019	4.176148	-0.000001
H	-0.000509	3.566652	-2.344118
H	2.459229	2.052665	-1.486696
H	2.459227	2.052665	1.486698
H	-0.000509	3.566654	2.344119
H	-0.000058	0.410767	2.481029
I	2.113769	-1.353236	0.000000
H	-0.000058	0.410767	-2.481030
H	-2.459815	2.051952	-1.486698
H	-2.459814	2.051952	1.486699
I	-2.113382	-1.353838	0.000000

</icarb_bp86_xyz>

<icarb_pbe0_xyz>

H	-4.128534	1.340679	-0.000001
C	-3.168597	0.847510	0.000000
C	-3.189350	-0.764661	0.000000
B	-2.763643	0.036209	-1.444060
B	-1.870226	1.457023	-0.888478
B	-1.870226	1.457022	0.888478

B	-2.763644	0.036209	1.444060
B	-1.004971	0.013265	1.449291
B	-0.444084	0.896224	0.000000
B	-1.004972	0.013265	-1.449291
B	-1.907350	-1.407509	-0.888558
B	-1.907350	-1.407509	0.888558
B	-0.467411	-0.884019	0.000000
H	-4.161744	-1.232819	-0.000001
H	-3.548118	0.046516	-2.326062
H	-2.011965	2.473038	-1.474763
H	-2.011965	2.473037	1.474764
H	-3.548119	0.046516	2.326063
H	-0.404654	0.005416	2.468180
I	1.372166	2.076787	0.000000
H	-0.404654	0.005416	-2.468181
H	-2.075480	-2.419507	-1.474839
H	-2.075480	-2.419506	1.474840
I	1.317226	-2.112010	0.000000

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