

Supporting Information: Understanding of the C-H stretching region of Infra-Red spectroscopy: An analysis of the final state wavefunctions.

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Table S1. The normal modes and harmonic wavenumbers of Pyrimidine

Mode No.	Symm.	Description	HO wavenumber
1	a ₁	sym. CH str.	3201.76
2	a ₁	sym. CH str.	3171.68
3	a ₁	sym. CH str.	3155.55
4	a ₁	H-C-C ip bend ¹ + H-C-N ip bend + C-N str.	1607.15
5	a ₁	H-C-N ip bend + H-C-C ip bend + C-H str.	1436.99
6	a ₁	H-C-N ip bend +N-C-N ip bend	1162.76
7	a ₁	C-N str. + C-C str. + H-C-C ip bend	1082.71
8	a ₁	ring breathing	1009.62
9	a ₁	N-C-N ip bend + C-C-C bend	696.90
10	a ₂	CH oop bend ¹	1002.99
11	a ₂	ring torsion	409.16
12	b ₁	CH oop bend	1027.72
13	b ₁	CH oop bend	984.19
14	b ₁	CH oop bend	822.34
15	b ₁	CH oop bend	737.71
16	b ₁	ring torsion	351.59
17	b ₂	asym. CH str.	3158.73
18	b ₂	C-C str. + H-C-C ip bend	1606.05
19	b ₂	H-C-C ip bend + H-C-N ip bend	1499.43
20	b ₂	H-C-C ip bend + H-C-N ip bend	1400.29
21	b ₂	H-C-C ip bend + H-C-N ip bend + C-N str.	1250.97
22	b ₂	C-C str. + C-N str.	1206.18
23	b ₂	H-C-C ip bend	1094.69
24	b ₂	C-C-N ip bend	637.75

¹ ip= in-plane; oop = out-of-plane

Table S2. The normal modes and harmonic wavenumbers of Thiophene

Mode No.	Symm.	Description	HO wavenumber
1	a ₁	sym. CH str.	3254.75
2	a ₁	sym. CH str.	3215.5
3	a ₁	C-C str. + H-C-C ip bend	1438.74
4	a ₁	H-C-C ip bend + H-C-S ip bend	1395.88
5	a ₁	H-C-C ip bend + H-C-S ip bend	1106.56
6	a ₁	C-C str.	1051.92
7	a ₁	C-S str.	834.45
8	a ₁	C-S-C ip bend + C-S str.	613.37
9	a ₂	CH oop bend	921.09
10	a ₂	CH oop bend	688.53
11	a ₂	ring torsion	579.08
12	b ₁	CH oop bend	888.39
13	b ₁	CH oop bend	722.95
14	b ₁	ring torsion	462,61
15	b ₂	asym. CH str.	3252.20
16	b ₂	asym. CH str.	3202.12
17	b ₂	C-C str. + H-C-C ip bend	1549.76
18	b ₂	H-C-C ip bend + H-C-S ip bend	1284.56
19	b ₂	H-C-C ip bend + H-C-S ip bend	1106.52
20	b ₂	C-C-C ip bend + H-C-S ip bend + C-C-S ip bend	877.81
21	b ₂	C-S str.	746.25

ip= in-plane; oop = out-of-plane

Table S3. The Cartesian coordinates (in Angstroms) of the optimized structure of pyrimidine, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
C	0.000000	0.000000	-1.308558
N	0.000000	1.192933	-0.712855
C	0.000000	1.181290	0.621569
C	0.000000	0.000000	1.350600
C	0.000000	-1.181290	0.621569
N	0.000000	-1.192933	-0.712855
H	0.000000	2.146274	1.115002
H	0.000000	0.000000	-2.391906
H	0.000000	0.000000	2.430795
H	0.000000	-2.146274	1.115002

Table S4. The Cartesian coordinates (in Angstroms) of the optimized structure of pyrimidine-d4, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
C	0.000000	0.000000	-1.308558
N	0.000000	1.192933	-0.712855
C	0.000000	1.181290	0.621569
C	0.000000	0.000000	1.350600
C	0.000000	-1.181290	0.621569
N	0.000000	-1.192933	-0.712855
D	0.000000	2.146274	1.115002
D	0.000000	0.000000	-2.391906
D	0.000000	0.000000	2.430795
D	0.000000	-2.146274	1.115002

Table S5. The Cartesian coordinates (in Angstroms) of the optimized structure of Thiophene, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
C	0.000000	1.238795	-0.010103
C	0.000000	0.712165	-1.268287
C	0.000000	-0.712165	-1.268287
C	0.000000	-1.238795	-0.010103
S	0.000000	0.000000	1.194166
H	0.000000	2.274830	0.280569
H	0.000000	1.315107	-2.163562
H	0.000000	-1.315107	-2.163562
H	0.000000	-2.274830	0.280569

Table S6. The Cartesian coordinates (in Angstroms) of the optimized structure of Thiophene-d4, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
C	0.000000	1.238795	-0.010103
C	0.000000	0.712165	-1.268287
C	0.000000	-0.712165	-1.268287
C	0.000000	-1.238795	-0.010103
S	0.000000	0.000000	1.194166
D	0.000000	2.274830	0.280569
D	0.000000	1.315107	-2.163562
D	0.000000	-1.315107	-2.163562
D	0.000000	-2.274830	0.280569

Table S7. The Cartesian coordinates (in Angstroms) of the optimized structure of pyrazine, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
C	0.000000	1.131088	0.696090
C	0.000000	1.131088	-0.696090
N	0.000000	0.000000	-1.401268
C	0.000000	-1.131088	-0.696090
C	0.000000	-1.131088	0.696090
N	0.000000	0.000000	1.401268
H	0.000000	2.060922	1.251864
H	0.000000	2.060922	-1.251864
H	0.000000	-2.060922	-1.251864
H	0.000000	-2.060922	1.251864

Table S8. The Cartesian coordinates (in Angstroms) of the optimized structure of pyrazine-d4, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
C	0.000000	1.131084	0.696090
C	0.000000	1.131084	-0.696090
N	0.000000	0.000000	-1.401261
C	0.000000	-1.131084	-0.696090
C	0.000000	-1.131084	0.696090
N	0.000000	0.000000	1.401261
D	0.000000	2.060930	1.251843
D	0.000000	2.060930	-1.251843
D	0.000000	-2.060930	-1.251843
D	0.000000	-2.060930	1.251843

Table S9. The Cartesian coordinates (in Angstroms) of the optimized structure of trans-butadiene, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
C	-0.325181	0.650343	0.000000
C	0.325181	1.816497	0.000000
H	-1.410504	0.646518	0.000000
H	-0.202410	2.759441	0.000000
H	1.407080	1.859005	0.000000
C	-0.325181	-1.816497	0.000000
C	0.325181	-0.650343	0.000000
H	0.202410	-2.759441	0.000000
H	-1.407080	-1.859005	0.000000
H	1.410504	-0.646518	0.000000

Table S10. The Cartesian coordinates (in Angstroms) of the optimized structure of trans-butadiene-d6, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
C	-0.325182	0.650344	0.000000
C	0.325182	1.816498	0.000000
D	-1.410504	0.646521	0.000000
D	-0.202410	2.759442	0.000000
D	1.407081	1.859004	0.000000
C	-0.325182	-1.816498	0.000000
C	0.325182	-0.650344	0.000000
D	0.202410	-2.759442	0.000000
D	-1.407081	-1.859004	0.000000
D	1.410504	-0.646521	0.000000

Table S11. The Cartesian coordinates (in Angstroms) of the optimized structure of pyridazine, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
N	0.000000	0.665768	-1.226446
C	0.000000	1.320475	-0.067334
C	0.000000	0.689189	1.175089
C	0.000000	-0.689189	1.175089
C	0.000000	-1.320475	-0.067334
N	0.000000	-0.665768	-1.226446
H	0.000000	1.265462	2.089594
H	0.000000	2.399637	-0.151001
H	0.000000	-1.265462	2.089594
H	0.000000	-2.399637	-0.151001

Table S12. The Cartesian coordinates (in Angstroms) of the optimized structure of pyridazine-d4, computed by B3LYP/6-311++G(2d,2p) method.

Atom	X	Y	Z
N	0.000000	0.665768	-1.226446
C	0.000000	1.320475	-0.067334
C	0.000000	0.689189	1.175089
C	0.000000	-0.689189	1.175089
C	0.000000	-1.320475	-0.067334
D	0.000000	-0.665768	-1.226446
D	0.000000	1.265462	2.089594
D	0.000000	2.399637	-0.151001
D	0.000000	-1.265462	2.089594
D	0.000000	-2.399637	-0.151001

S1. PYRAZINE

Twenty four normal modes of Pyrazine are tabulated in Table S13 along with their symmetry representations, approximate physical descriptions, and harmonic wavenumbers. Out of four CH stretching fundamentals, only two are (9_1 and 15_1) IR active, and they belong to b_{1u} and b_{2u} irreducible representations of the D_{2h} point group, respectively. A comparison between the experimental spectrum and the computed spectrum of the CH stretching region is presented in Figure S1. The experimental spectrum is taken from the NIST database. The calculated results are convoluted with a gaussian line shape function of 20 cm^{-1} FWHM bandwidth and presented along with the stick spectrum underneath it. As can be seen, there is good agreement between the experimental spectrum and the computed one. The experimental spectrum has five bands in the CH stretching region that are spread over 2900 to 3100 cm^{-1} . We found four bands in this region in our computation. The experimental band, labeled as 1, is reproduced by the VCCM calculation. The intensity of the computed band is overestimated as compared to the experimental one. As can be seen from the stick spectrum, this calculated band is the superposition of two medium and several low-intensity transitions. The bands 2 and 3 of the experimental spectrum have been merged into a single band in the calculated spectrum (labeled as 2). This band is the superposition of one medium and several low-intensity transitions. The band 4 of the computed spectrum mimics the band 4 of the experimental spectrum. The stick spectrum shows that this band is the superposition of one high intensity and one medium intensity transitions. The computed band 5 is a superposition of several low-intensity transitions that may be assigned as the shoulder peak 5 of the experimental spectrum. We found an additional band, marked as 0, at the lower end of the band 1 in our calculations.

The redistribution of intensities of the zeroth-order fundamental transitions over several transitions in the anharmonic calculations is observed for the Pyrazine molecule also. A total of eighteen transitions with intensities more than 0.30 km.mol^{-1} are listed in table S14. The transition energies are distributed within the about 260 cm^{-1} of energy region. Several transitions are clustered together within a small energy region. Such clustering of the transitions are also found in Pyrimidine and Thiophene molecule, as discussed in the main text. These clustered transitions have comparable molar extinction coefficients. For example, the transitions 2-4 of the b_{2u} representation are clustered together within 4 cm^{-1} energy, between 2951 to 2955 cm^{-1} . The molar extinction coefficients of these transitions vary between 9.61 to 1.13 km.mol^{-1} . Similarly, the transitions 6 and 7 of the same b_{2u} representation are clustered together within 2 cm^{-1} . The molar extinction coefficients of these two transitions are 18.11 and 5.25 km.mol^{-1} , respectively.

All the four transitions of b_{1u} and fourteen transitions of b_{2u} representation borrowed intensities predominantly from 9_1 and 15_1 CH stretch chromophores, respectively. We recall that a similar situation is observed in the b_2 representation of pyrimidine where all the transitions received intensities from the asymmetric CH stretch chromophore. Since it is the only primary chromophore present in this representation, the ratio of the intensity to the weight of the zeroth-order CH stretch in the final states of the transitions was found to be a constant. For the pyrazine also we find that the ratio of the intensity of a transition to the weight of the zeroth-order CH stretch fundamental (I_i/w_i) is nearly constant for each symmetry. For example, such the ratio is about 2.4 for the transitions in b_{1u} representation. For the most intense transition of b_{2u} representation, the (I_i/w_i) value is about 65. The value of such a ratio is also 65 for transitions 1 and 7. We note that several intense transitions (transitions 2-5 and 10) do not have 15_1 chromophore as the most or second most important zeroth-order state in their final wavefunctions. With a more detail analysis of these final state wavefunctions, we find that the zeroth-order 15_1 state appears as the third or fourth most significant zeroth-order states in these wavefunctions. The ratio of intensity to the weight of 15_1 fundamental is about 65 for all these transitions.

The final states of the transitions are superpositions of several zeroth-order states. In nine of these states, the weight of the most important zeroth-order state is less than 50%. Several zeroth-order states have near equal contributions in the final states of many of these transitions. Consequently, these states cannot be described by a single zeroth-order state alone. For example, in the final state of the third transition of b_{1u} representation, the most significant zeroth-order state, $23_114_17_16_1$, has 37% weight and the second most contributing state (9_1) has 27% weight. Similarly, the final state of transition 2 of b_{2u} representation receives only 36% contribution from its most significant zeroth-order state $23_111_17_15_1$ and 29% contribution from the second most important zeroth-order state 16_12_1 .

The final states are dominated by three or four quantum excitations for most of the transitions listed here. Nine of these transitions have a four quantum state as the most dominating configuration in their final states, and four of the states have a four quantum state as the second most contributing zeroth-order state. Four of the final states have a three quantum state as the most significant zeroth-order state.

The contribution of the primary chromophores CH stretch is significantly small in the states reported here. In all the transitions of b_{1u} representation, the primary chromophore 9_1 is the second most significant zeroth-order state. The highest contribution from 9_1 is only 27% in the final state of transition 3 of this irreducible representation. We note that the primary chromophore 15_1 has the most significant contribution in the final state of transition 6 of b_{2u}

representation, which is only 28%. Thus, none of the transitions can be characterized as a fundamental transition.

Table S13. The normal modes and harmonic wavenumbers of Pyrazine

Mode No.	Symm.	Description	HO wavenumber
1	a_g	sym. CH str.	3176.09
2	a_g	C-C str.	1612.14
3	a_g	H-C-C ip bend + H-C-N ip bend	1253.07
4	a_g	C-C str. + C-N str.	1038.99
5	a_g	C-N-C ip bend	615.07
6	a_u	H-C-C oop bend	1005.85
7	a_u	ring torsion	351.46
8	b_{1g}	H-C-C oop bend	944.94
9	b_{1u}	CH str.	3156.26
10	b_{1u}	H-C-C ip bend + H-C-N ip bend	1518.68
11	b_{1u}	H-C-N ip bend	1164.79
12	b_{1u}	C-N-C ip bend	1037.75
13	b_{2g}	H-C-C oop bend	993.17
14	b_{2g}	ring twisting	778.40
15	b_{2u}	CH str.	3170.19
16	b_{2u}	H-C-N ip bend + H-C-C ip bend	1445.53
17	b_{2u}	C-C str. + C-N str.	1208.13
18	b_{2u}	C-C str. + H-C-C ip bend	1089.51
19	b_{3g}	CH str.	3155.11
20	b_{3g}	C-N str.	1575.71
21	b_{3g}	H-C-N ip bend + H-C-C ip bend	1378.76
22	b_{3g}	C-C-N ip bend	720.70
23	b_{3u}	H-C-C oop bend	803.61
24	b_{3u}	ring torsion	433.77

ip= in-plane; oop = out-of-plane

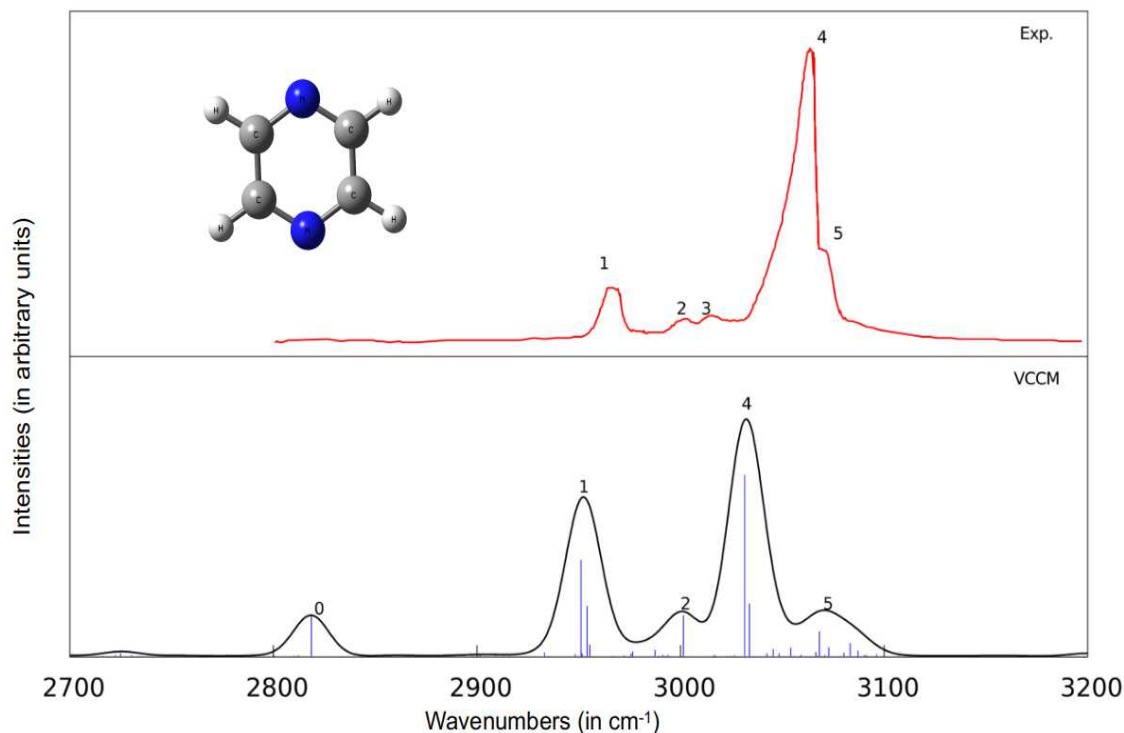


Figure S1. The CH stretching region of IR spectra of pyrazine. The VCCM spectra is convoluted with a gaussian line shape function of 20 cm^{-1} FWHM, and the corresponding stick spectrum is presented along with it. The gas phase experimental spectrum is taken from NIST database.

Table S14. Some bright states of Pyrazine in the CH stretching region. Transitions with intensities more than 0.30 km.mol^{-1} are tabulated.

Symmetry	Transition no.	Excitation energy	State description	Intensity
b_{1u}	1	2933.18	$0.73*20_116_1+0.14*9_1$	0.37
	2	2976.45	$0.41*23_114_17_16_1+0.19*9_1$	0.44
	3	2987.47	$0.37*23_114_17_16_1-0.27*9_1$	0.61
	4	3066.39	$0.53*10_12_1-0.18*9_1$	0.42
b_{2u}	1	2818.63	$0.82*21_110_1-0.06*15_1$	3.99
	2	2951.07	$0.36*23_111_17_15_1+0.29*16_12_1$	9.61
	3	2954.12	$0.55*23_111_17_15_1-0.20*16_12_1$	5.01
	4	2955.38	$0.45*22_112_13_1-0.35*22_112_15_2$	1.13
	5	3001.43	$0.63*20_110_1-0.16*16_12_1$	4.07
	6	3031.57	$0.28*15_1+0.16*20_110_1$	18.11
	7	3033.82	$0.63*13_111_18_1-0.08*15_1$	5.25
	8	3045.42	$0.46*24_123_117_15_1-0.28*16_15_14_1$	0.67
	9	3054.07	$0.89*14_18_27_1-0.01*15_1$	0.84
	10	3068.23	$0.36*23_121_113_1-0.23*23_213_17_1$	2.46
	11	3072.77	$0.73*23_120_114_1-0.09*23_121_113_1$	0.87
	12	3080.28	$0.63*22_111_15_2+0.15*21_111_15_1$	0.32
	13	3083.33	$0.29*24_123_28_1-0.19*23_213_17_1$	1.30
	14	3087.11	$0.43*24_123_28_1+0.13*23_122_117_17_1$	0.53

S2. TRANS-BUTADIENE

Trans-butadiene is an open-chain molecule in our analysis. Twenty four normal modes span as $9a_g+4a_u+3b_g+8b_u$ in the irreducible representation of C_{2h} point group. The approximate descriptions of the normal modes, symmetry representations, and the harmonic wavenumbers are presented in table S15. Out of six CH stretch fundamentals, only three are IR active and they all belong to b_u representation.

The experimental spectrum of the CH stretch region is compared with the computed spectrum by the VCCM method in figure S2. The computed spectrum is convoluted with 20 cm^{-1} gaussian bandwidth. We presented the stick spectrum underneath of the convoluted spectrum for comparison. Overall, the experimental spectrum is fairly well reproduced by the VCCM. The experimental spectrum is broad, spans over 2950 to 3150 cm^{-1} region, and has seven bands. We found several transitions in this region, as reported in the stick spectrum. With 20 cm^{-1} bandwidth, these transitions generate six bands. The experimental band, labeled as 1, is simulated as band 1 in the VCCM calculations. However, the intensity of the computed band is significantly underestimated. The band 2 of the computed spectrum represents the band 2 of the experimental spectrum. This band is the superposition of one high-intensity transition and several medium and low-intensity transitions. The band 6 and 7 of the experimental spectrum are merged into one band (labeled as 5) in the anharmonic calculations.

The intensities of three CH stretch fundamentals are distributed over several transitions in the small energy region, and this leads to a broad structure of the experimental spectrum in the CH stretch region. There are as many as thirty-four transitions with intensity more than 0.30 km.mol^{-1} . These transitions are listed in table S16. These transitions span over 190 cm^{-1} of energy.

The general features of the transitions in the CH stretch region of this molecule are similar to the other molecules under study. Here also, we found clustering of several transitions within the small energy region, and the clustered transitions have comparable molar extinction coefficients. For example, the transitions 7-11 are clustered together within 8 cm^{-1} , between 2958 to 2966 cm^{-1} . The molar extinction coefficients of these transitions vary between 0.45 to 2.79 km.mol^{-1} .

Several zeroth-order states have significant contributions in the final state wavefunctions of the transitions in the CH stretch region. In twenty-five out of thirty-four transitions, the most significant zeroth-order states have less than 50% weight in their final states. Several zeroth-order states have near equal contributions in the final states of these transitions, implying that these states can not be described by a single zeroth-order state alone. For example, for the transition 2, both the most significant zeroth-order state ($14_112_15_1$) and the second most important zeroth-order state ($20_113_112_19_1$) have only 14% weight. Several other zeroth-order states constitute the rest of 72% of the wavefunction.

Like other molecules in this study, the final states of the transitions are mostly dominated by three and/or four quantum zeroth-order states. The contributions of the primary CH chromophores are significantly small in these transitions, and they mix strongly with three and/or four quantum states due to near degeneracy. The maximum contribution from the primary chromophore is found in transition 6, where 19_1 has only 24% weight in the final state. Notably, this is the most intense transition reported here. The second most important zeroth-order state of the final state of this transition is a four quantum state ($16_115_114_113_1$) with 13% weight. The chromophore 18_1 is not the most significant zeroth-order state in the final state any of the transitions. It is the second most significant zeroth-order state in the final state of transition 14 with 13% weight. The most important zeroth-order state of the final state of this transition is a four quantum state ($16_114_213_1$) and it has 27% weight. The primary chromophore 17_1 is the most significant zeroth-order state in the final state of transition 28, and its weight is only 21%. The second most contributing zeroth-order state is again a four quantum state (24_18_3) with 15% weight in the final state of this transition.

Table S15. The normal modes and harmonic wavenumbers of trans-butadiene

Mode No.	Symm.	Description	HO wavenumber
1	a_g	sym. CH str.	3225.98
2	a_g	sym. CH str.	3141.91
3	a_g	sym. CH str.	3130.46
4	a_g	C=C str.	1698.03
5	a_g	CH2 scis.	1481.68
6	a_g	H-C-C ip bend	1319.62
7	a_g	C-C str.	1229.77
8	a_g	CH2 rock	900.39
9	a_g	C-C-C ip bend	519.29
10	a_u	H-C-C oop bend	1053.02
11	a_u	H-C-C oop bend	941.12
12	a_u	H-C-C oop bend	538.56
13	a_u	CCC deform	172.96
14	b_g	H-C-C oop bend	1000.01
15	b_g	H-C-C oop bend	940.27
16	b_g	H-C-C oop bend	779.07
17	b_u	asym. CH str.	3226.37
18	b_u	asym. CH str.	3143.18
19	b_u	asym. CH str.	3139.30
20	b_u	C=C str.	1647.75
21	b_u	CH2 scis.	1420.50
22	b_u	H-C-C ip bend	1327.12
23	b_u	CH2 rock	1010.36
24	b_u	C-C-C ip bend	298.89

ip= in plane; oop = out-of-plane

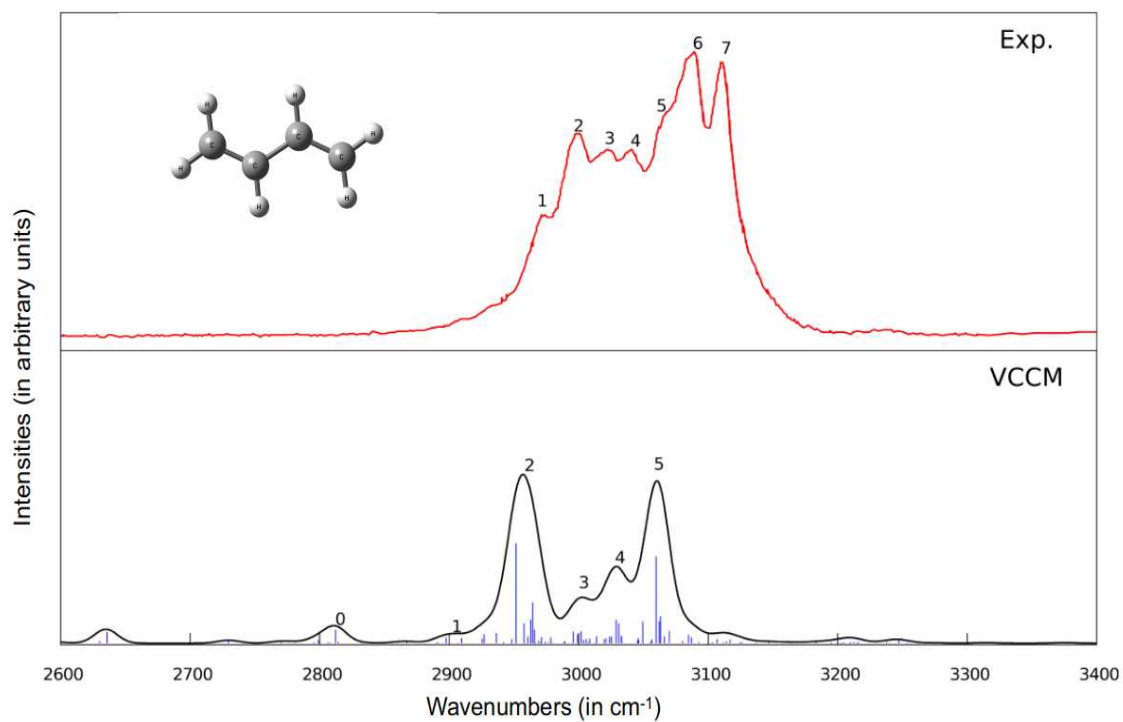


Figure S2. The CH stretching region of IR spectra of trans-butadiene. The VCCM spectra is convoluted with a gaussian line shape function of 20 cm^{-1} FWHM, and the corresponding stick spectrum is presented along with it. The gas phase experimental spectrum is taken from NIST database.

Table S16. Some bright states of trans-butadiene in the CH stretching region. Transitions with intensities more than 0.30 km.mol^{-1} are tabulated here.

Symmetry	Transition no.	Excitation energy	State description	Intensity
b_u	1	2897.69	$0.46*21_112_110_1 - 0.27*24_112_110_18_1$	0.38
	2	2909.64	$0.14*14_112_15_1 + 0.14*20_113_112_19_1$	0.35
	3	2925.34	$0.45*23_114_2 - 0.09*14_112_15_1$	0.30
	4	2927.11	$0.37*22_14_1 + 0.09*20_16_1$	0.62
	5	2936.44	$0.38*24_17_15_1 - 0.11*22_14_1$	0.70
	6	2951.58	$0.24*19_1 + 0.13*16_115_114_113_1$	6.82
	7	2957.84	$0.67*16_113_19_15_1 - 0.05*19_1$	1.35
	8	2960.86	$0.25*22_116_115_1 + 0.22*24_221_8_1$	0.45
	9	2962.88	$0.41*24_221_8_1 - 0.22*22_116_115_1$	1.62
	10	2964.41	$0.23*16_110_17_1 + 0.15*16_111_6_1$	2.79
	11	2965.81	$0.41*16_110_17_1 - 0.16*16_115_114_113_1$	0.95
	12	2971.33	$0.50*15_113_19_16_1 - 0.21*22_113_26_1$	0.41
	13	2978.40	$0.50*24_123_114_112_1 + 0.07*20_112_111_1$	0.39
	14	2995.83	$0.27*16_114_213_1 - 0.13*18_1$	0.79
	15	2999.06	$0.73*14_113_18_2 - 0.07*18_1$	0.61
	16	3001.84	$0.31*16_114_213_1 + 0.09*18_1$	0.81
	17	3008.44	$0.29*16_113_111_10_1 - 0.13*16_312_1$	0.32
	18	3013.86	$0.55*22_19_17_1 + 0.09*23_113_112_17_1$	0.48
	19	3021.18	$0.57*23_110_2 + 0.23*22_116_114_1$	0.33
	20	3023.88	$0.73*23_216_113_1 + 0.07*24_16_15_1$	0.46
	21	3025.38	$0.35*24_16_15_1 - 0.20*23_216_113_1$	0.46
	22	3028.93	$0.25*15_111_17_1 - 0.14*24_16_15_1$	1.61
	23	3030.93	$0.43*15_111_17_1 + 0.07*23_113_112_17_1$	1.36
	24	3032.93	$0.38*24_113_110_15_1 + 0.13*24_116_114_18_1$	0.51
	25	3033.20	$0.27*21_14_1 - 0.21*24_113_110_15_1$	0.40
	26	3045.99	$0.63*24_122_116_112_1 - 0.13*14_112_19_18_1$	0.33
	27	3049.44	$0.39*20_15_1 - 0.15*14_112_19_18_1$	1.47
	28	3059.81	$0.21*17_1 - 0.15*24_18_3$	5.93
	29	3062.29	$0.47*24_18_3 - 0.11*24_121_2$	1.49
	30	3063.18	$0.29*24_121_2 + 0.24*21_116_115_1$	1.82
	31	3066.25	$0.49*22_18_2 - 0.07*24_19_18_16_1$	0.46
	32	3069.90	$0.36*23_113_111_18_1 - 0.16*15_113_111_2$	0.86
	33	3084.78	$0.74*24_120_115_113_1 + 0.07*23_18_17_1$	0.58
	34	3087.16	$0.43*16_112_210_1 - 0.14*20_112_110_1$	0.40

S3. PYRIDAZINE

Twenty four normal modes of Pyridazine span as $9a_1 + 4a_2 + 3b_1 + 8b_2$ in the irreducible representations of C_{2v} point group. The approximate descriptions of the normal modes, symmetry representations, and the harmonic wavenumbers are presented in table S17. All the CH stretch are IR active. The comparison between the experimental spectrum and the computed spectrum is presented in figure S3. The experimental spectrum is taken from the NIST database. The experimental spectrum is in the liquid phase while the computation assumes the gas phase at absolute temperature. Thus, the comparison between them is not very apt since the intermolecular interactions that affect the bandwidth significantly are not considered here. Despite that, the computed spectrum described the experimental spectrum fairly well.

Four transitions of a_1 representation and nine transitions of b_2 representation that have molar extinction coefficient values more than 0.30 km.mol^{-1} are listed in table S18. The transitions of a_1 representation receive intensities from zeroth-order 1_1 and 2_1 fundamentals, and transitions of the b_2 representation receive intensities from 17_1 and 18_1 fundamentals, respectively. These transitions are spread over about 190 cm^{-1} energy range between 2947 to 3132 cm^{-1} .

The strong mixing of the multi-quantum zeroth-order states with the CH stretch fundamentals due to near degeneracy leads to extensive intensity redistribution from the CH stretching fundamentals to several other transitions in the anharmonic description. In the many-body description of the wave-functions of the final states of these transitions, the weights of the zeroth-order CH stretch fundamentals are significantly small and they mix strongly with multi-quantum zeroth-order states. Consequently, the multi-quantum zeroth-order states have significant weights in these functions. None of these final states has more than 50% contribution from any of the zeroth-order CH stretch fundamental, implying that none of the transitions can strictly be termed as the fundamental transition. For example, 1_1 state is the most significant zeroth-order state in the final state of transition 1 of a_1 representation. However, its weight is only 26%. It is the second most important zeroth-order state of the other three transitions. The total weight of 1_1 fundamental in all these four final states is 55%. The rest 45% of this zeroth-order state are distributed over several final states and each will receive small intensity from the 1_1 fundamental. None of the transition tabulated here has 2_1 fundamental as the most important configuration. It is the second most important zeroth-order state in the final state of transition 1 with 17% weight. We note that the harmonic intensity of 1_1 is about 1000 times more than 2_1 , and thus the transitions of a_1 irreducible representation receive intensities mainly from 1_1 fundamental.

Such features of the many-body wave-functions of the final states of the transitions are persistent for b_2 representation as well. Only for the final state of transition 7, the primary chromophore 17_1 is the most important configuration with 37% weight. Consequently, this is the most intense transition of this representation. None of the transition has 18_1 as the most or second most significant state in their final state wave-functions.

The final states of most of the transitions tabulated here have a four quantum or three quantum zeroth-order state as the most or the second most important zeroth-order states. The weight of these states is usually small (less than half) in all most all the transitions reported here. Consequently, these state cannot be assigned by a single zeroth-order state in the accurate description.

Table S17. The normal modes and harmonic wave-numbers of Pyridazine

Mode No.	Symm.	Description	HO wavenumber
1	a ₁	sym. CH str.	3200.70
2	a ₁	sym. CH str.	3175.15
3	a ₁	C-C str. + H-C-C ip bend	1608.51
4	a ₁	H-C-N ip bend + H-C-C ip bend	1481.59
5	a ₁	H-C-C ip bend	1177.35
6	a ₁	C-N str. + N-N str. + H-C-C ip bend	1173.32
7	a ₁	N-N str + C-C str. + H-C-C ip bend	1089.18
8	a ₁	N-N str + C-C str.	1005.92
9	a ₁	N-C-C ip bend	682.93
10	a ₂	H-C-C oop bend	1018.23
11	a ₂	H-C-C oop bend	942.76
12	a ₂	H-C-C oop bend + H-C-N oop bend	773.45
13	a ₂	ring torsion	376.36
14	b ₁	H-C-C oop bend	984.70
15	b ₁	H-C-C oop bend	760.71
16	b ₁	ring torsion	374.69
17	b ₂	asym. CH str.	3187.76
18	b ₂	asym. CH str.	3170.55
19	b ₂	C-N str. + C-C str. + H-C-N ip bend + H-C-C ip bend	1602.53
20	b ₂	H-C-C ip bend	1446.62
21	b ₂	H-C-N ip bend + H-C-C ip bend	1314.98
22	b ₂	H-C-C ip bend	1086.60
23	b ₂	C-N-N ip bend + C-C-C ip bend + H-C-C ip bend	1062.87
24	b ₂	C-C-C ip bend + C-C-N ip bend	637.32

ip= in-plane; oop = out-of-plane

Table S18. Some bright states of pyridazine in the CH stretching region. Transitions with intensities more than 0.30 km.mol⁻¹ are tabulated.

Symmetry	Transition no.	Excitation energy	State description	Intensity
a ₁	1	3033.94	0.26*1 ₁ +0.17*2 ₁	2.33
	2	3037.12	0.61*24 ₁ 21 ₁ 6 ₁ +0.09*1 ₁	0.71
	3	3046.37	0.22*15 ₂ 3 ₁ -0.19*1 ₁	1.32
	4	3131.68	0.80*3 ₂ +0.06*1 ₁	0.30
b ₂	1	2946.77	0.46*14 ₁ 13 ₁ 12 ₂ +0.13*20 ₁ 3 ₁	0.44
	2	2948.55	0.38*20 ₁ 3 ₁ -0.18*14 ₁ 13 ₁ 12 ₂	0.89
	3	2959.06	0.34*24 ₁ 13 ₁ 12 ₁ 5 ₁ -0.09*15 ₁ 12 ₁ 4 ₁	0.34
	4	2970.82	0.28*16 ₁ 10 ₁ 3 ₁ +0.12*19 ₁ 4 ₁	1.63
	5	2977.82	0.18*19 ₁ 13 ₁ 10 ₁ -0.14*16 ₁ 15 ₁ 14 ₁ 12 ₁	0.72
	6	3050.28	0.51*24 ₁ 8 ₁ 4 ₁ -0.14*24 ₁ 23 ₁ 14 ₁ 13 ₁	0.56
	7	3062.56	0.37*17 ₁ -0.18*19 ₁ 4 ₁	11.48
	8	3086.33	0.24*15 ₁ 11 ₁ 4 ₁ -0.22*16 ₁ 15 ₂ 10 ₁	0.54
	9	3088.63	0.33*16 ₁ 15 ₁ 210 ₁ +0.16*15 ₁ 11 ₁ 4 ₁	0.82

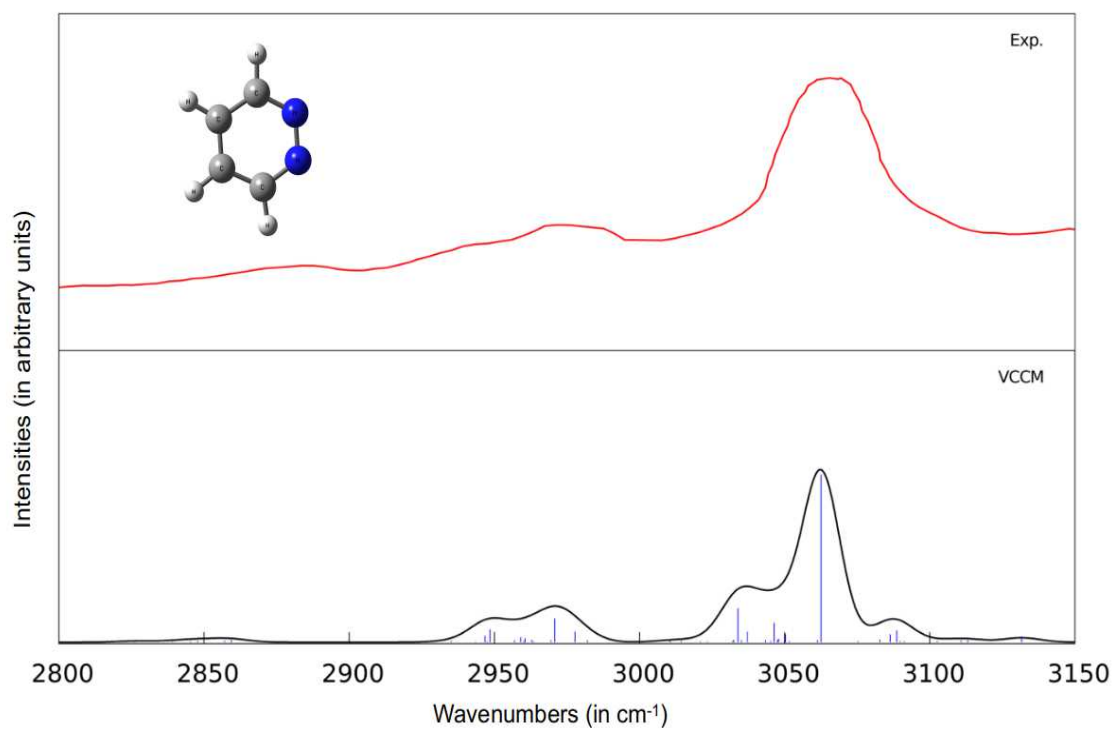


Figure S3. The CH stretching region of IR spectra of pyridazene. The VCCM spectra is convoluted with a gaussian line shape function of 15 cm⁻¹ FWHM, and the corresponding stick spectrum is presented along with it. The liquid phase experimental spectrum is taken from NIST database.

Table S19. Transitions in the CD stretching region of pyrimidine-d4. Transitions with intensities more than 0.50 km.mol⁻¹ are tabulated here.

Symmetry	Transition no.	Excitation energy	State description	Intensity
a ₁	1	2238.95	0.40*21 ₁ 13 ₁ 11 ₁ -0.11*22 ₁ 19 ₁	0.79
	2	2242.50	0.81*24 ₁ 13 ₁ 10 ₁ +0.05*15 ₁ 13 ₁ 8 ₁	0.61
	3	2244.85	0.46*3 ₁ -0.17*7 ₁ 5 ₁	11.70
	4	2256.97	0.58*7 ₁ 5 ₁ +0.13*3 ₁	2.31
	5	2274.39	0.34*2 ₁ -0.25*14 ₁ 13 ₁ 11 ₂	3.11
	6	2275.86	0.31*14 ₁ 13 ₁ 11 ₂ +0.19*2 ₁	0.81
	7	2289.94	0.70*1 ₁ +0.06*23 ₁ 18 ₁	5.79
b ₂	1	2253.91	0.56*24 ₁ 9 ₁ 7 ₁ -0.26*17 ₁	5.09
	2	2255.15	0.31*24 ₁ 9 ₁ 7 ₁ -0.29*24 ₂ 21 ₁	3.73
	3	2256.28	0.64*24 ₂ 21 ₁ -0.11*13 ₁ 11 ₁ 6 ₁	1.62
	4	2258.35	0.43*13 ₁ 11 ₁ 6 ₁ +0.19*17 ₁	3.70
	5	2316.95	0.73*21 ₁ 5 ₁ -0.11*12 ₁ 10 ₁ 9 ₁	0.90
	6	2448.00	0.57*20 ₁ 5 ₁ - 0.13*13 ₁ 11 ₁ 5 ₁	0.58

Table S20. Some bright states of thiophene-d4 in the CD stretching region. Transitions with intensities more than 0.10 km.mol⁻¹ are tabulated.

Symmetry	Transition no.	Excitation energy	State description	Intensity
a ₁	1	2290.68	0.40*14 ₁ 13 ₁ 8 ₁ 7 ₁ +0.28*2 ₁	0.20
	2	2290.91	0.56*14 ₁ 13 ₁ 8 ₁ 7 ₁ -0.23*2 ₁	0.16
	3	2323.02	0.23*20 ₁ 14 ₁ 10 ₁ 8 ₁ +0.17*1 ₁	0.19
	4	2328.84	0.28*11 ₂ 10 ₁ 9 ₁ +0.23*1 ₁	0.21
	5	2333.56	0.32*14 ₁ 13 ₁ 10 ₁ 9 ₁ -0.28*1 ₁	0.29
b ₂	1	2281.13	0.70*16 ₁ +0.03*18 ₁ 3 ₁	1.14

Table S21. Some bright states of trans-butadiene-D6 in the CD stretching region. Transitions with intensities more than 0.30 km.mol⁻¹ are tabulated here.

Symmetry	Transition no.	Excitation energy	State description	Intensity
b _u	1	2190.70	0.80*24 ₁ 15 ₂ 9 ₁ - 0.04*22 ₁ 9 ₁ 8 ₁	0.33
	2	2191.91	0.31*22 ₁ 9 ₁ 8 ₁ - 0.21*19 ₁	1.68
	3	2199.36	0.80*22 ₁ 16 ₂ - 0.05*24 ₁ 12 ₁ 11 ₁ 8 ₁	0.40
	4	2207.98	0.35*19 ₁ + 0.24*22 ₁ 5 ₁	4.75
	5	2213.82	0.54*14 ₁ 13 ₁ 12 ₁ 10 ₁ + 0.11*16 ₂ 14 ₁ 13 ₁	1.05
	6	2234.04	0.37*21 ₁ 9 ₁ 8 ₁ + 0.21*18 ₁	0.48
	7	2263.81	0.61*16 ₁ 13 ₁ 8 ₂ - 0.18*20 ₁ 8 ₁	0.37
	8	2269.11	0.39*20 ₁ 8 ₁ + 0.23*16 ₁ 13 ₁ 8 ₂	1.18
	9	2308.35	0.57*22 ₁ 16 ₁ 15 ₁ + 0.19*24 ₁ 22 ₁ 21 ₁	0.36
	10	2310.33	0.47*17 ₁ + 0.10*23 ₁ 4 ₁	5.54
	11	2351.26	0.62*23 ₁ 4 ₁ - 0.12*17 ₁	1.40

Table S22. Some bright states of Pyrazine-d4 in the CD stretching region. Transitions with intensities more than 0.30 km.mol⁻¹ are tabulated.

Symmetry	Transition no.	Excitation energy	State description	Intensity
b _{1u}	1	2205.64	0.53*21 ₁ 17 ₁ + 0.18*9 ₁	0.41
	2	2226.41	0.42*10 ₁ 4 ₁ - 0.21*9 ₁	0.54
	3	2251.33	0.32*10 ₁ 4 ₁ + 0.26*9 ₁	0.62
b _{2u}	1	2144.69	0.88*16 ₁ 4 ₁ + 0.05*13 ₁ 7 ₁ 3 ₁	0.54
	2	2233.58	0.73*23 ₂ 14 ₁ 7 ₁ - 0.07*23 ₁ 21 ₁ 14 ₁	2.81
	3	2249.99	0.70*15 ₁ - 0.09*16 ₁ 3 ₁	35.41
	4	2259.89	0.92*24 ₁ 11 ₁ 6 ₁ + 0.02*24 ₁ 8 ₁ 7 ₁ 6 ₁	0.49
	5	2274.71	0.65*24 ₁ 23 ₁ 16 ₁ - 0.13*16 ₁ 3 ₁	2.12
	6	2277.70	0.38*16 ₁ 3 ₁ + 0.33*14 ₃ 7 ₁	1.59
	7	2278.11	0.34*14 ₃ 7 ₁ - 0.32*16 ₁ 3 ₁	1.11
	8	2287.06	0.74*24 ₁ 21 ₁ 13 ₁ - 0.16*23 ₁ 21 ₁ 14 ₁	0.37
	9	2355.31	0.90*18 ₁ 2 ₁ + 0.02*18 ₁ 5 ₁ 4 ₁	0.44
	10	2386.71	0.87*21 ₁ 10 ₁ - 0.04*20 ₁ 12 ₁	0.69

Table S23. Some bright states of pyridazine-d4 in the CD stretching region. Transitions with intensities more than 0.30 km.mol^{-1} are tabulated.

Symmetry	Transition no.	Excitation energy	State description	Intensity
a ₁	1	2254.88	0.56*22 ₁ 20 ₁ +0.10*16 ₂ 12 ₁ 10 ₁	0.37
	2	2277.18	0.62*6 ₁ 4 ₁ +0.08*1 ₁	0.47
	3	2292.22	0.56*16 ₂ 14 ₂ -0.22*1 ₁	0.93
	4	2292.72	0.36*16 ₂ 14 ₂ +0.28*1 ₁	1.16
	5	2293.99	0.67*24 ₁ 21 ₁ 9 ₁ +0.11*1 ₁	0.44
b ₂	1	2247.77	0.67*18 ₁ +0.10*22 ₁ 4 ₁	5.81
	2	2264.46	0.53*15 ₁ 11 ₁ 6 ₁ -0.29*17 ₁	3.34
	3	2271.00	0.85*24 ₁ 13 ₂ 6 ₁ -0.05*17 ₁	0.54
	4	2271.28	0.28*17 ₁ +0.27*15 ₁ 11 ₁ 6 ₁	3.32
	5	2307.12	0.53*22 ₁ 4 ₁ -0.11*16 ₁ 10 ₁ 5 ₁	2.22
	6	2310.03	0.51*16 ₁ 10 ₁ 5 ₁ -0.10*14 ₁ 12 ₁ 8 ₁	0.30

Table S24. The linear dipole moment surface of Pyrimidine. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol^{-1}}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	2.83656D-10	-1.80471D-07	2.95331D+00
2	-2.08923D-10	-2.93293D-07	-3.61307D+00
3	2.63710D-10	3.12928D-08	-3.63641D+00
4	1.23171D-10	-2.40245D-07	6.49360D+00
5	2.36286D-10	6.16420D-08	-7.81283D+00
6	-1.81331D-10	5.04235D-08	1.21769D+00
7	-1.79063D-10	-1.29014D-09	-1.06905D+00
8	-3.92581D-10	1.74801D-08	1.91001D+00
9	4.73865D-11	-5.87210D-08	1.68820D+00
10	-2.67703D-08	-2.66811D-10	4.44194D-11
11	1.45697D-08	-4.01992D-11	-1.31558D-10
12	-3.14559D-02	5.93876D-10	5.33593D-10
13	1.96942D-01	-2.35263D-10	-4.78004D-10
14	-2.24483D+00	-1.04794D-09	-7.94407D-10
15	-6.48774D+00	-7.52315D-10	-4.76897D-10
16	1.88824D+00	-1.50869D-10	7.73198D-10
17	3.61124D-10	-3.33831D+00	-3.73874D-09
18	5.62090D-10	1.76910D+00	4.46235D-08
19	6.40468D-11	1.98429D+00	1.28477D-09
20	9.79945D-11	3.22771D+00	-2.40878D-09
21	3.05044D-11	6.09661D-01	1.32634D-08
23	2.10780D-10	-2.43151D+00	-4.06578D-08
23	1.15254D-10	-9.13585D+00	-1.77550D-07
24	1.20110D-10	4.15021D+00	-1.10089D-07

Table S25. The linear dipole moment surface of Pyrimidine-d4. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol^{-1}}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	-2.13414D-10	-1.15506D-07	2.13335D+00
2	5.61756D-11	-2.00472D-07	-3.33871D+00
3	3.14523D-11	1.14232D-08	-3.93762D+00
4	1.62799D-10	2.47260D-07	8.32947D+00
5	-1.22420D-11	3.65664D-08	-4.91525D+00
6	4.83524D-10	1.77454D-08	1.26287D+00
7	6.10408D-11	4.15530D-08	1.83847D+00
8	7.95066D-11	-1.09718D-08	-1.10532D+00
9	1.88852D-10	5.27686D-08	-1.72226D+00
10	-6.89316D-08	-5.42117D-11	-9.34564D-11
11	4.57694D-09	5.82335D-11	-6.20979D-10
12	1.50298D+00	7.33362D-11	7.25469D-11
13	1.08574D+00	-4.39662D-10	2.24789D-11
14	2.67872D-01	1.64044D-10	1.79881D-09
15	-4.81997D+00	-1.27050D-09	1.29600D-10
16	-1.78936D+00	-1.41506D-10	-6.53612D-11
17	2.56306D-10	4.38566D+00	-8.06781D-08
18	-1.66724D-10	9.43327D+00	-2.30898D-07
19	5.91203D-10	1.18176D-01	-1.79384D-08
20	-1.69468D-10	-2.21616D-01	8.74880D-10
21	-1.26519D-10	1.37620D-01	4.80666D-08
22	-2.11911D-10	-2.16329D+00	-5.96105D-09
23	4.27716D-11	1.57529D+00	2.63140D-10
24	-2.20873D-10	-3.23254D+00	-1.75716D-09

Table S26. The linear dipole moment surface of Pyridazene. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol^{-1}}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	-5.12756D-11	2.18171D-08	2.71541D+00
2	-7.75061D-11	-4.57508D-08	2.68191D-01
3	-1.62207D-12	-7.21655D-09	2.10959D+00
4	-1.13268D-11	7.76064D-08	-9.56666D-01
5	5.10583D-11	-2.21186D-08	-4.14836D-02
6	-7.64472D-11	-2.09656D-08	1.22625D-01
7	-1.10787D-10	-1.51781D-09	-3.37559D+00
8	8.15220D-11	3.90624D-08	2.76379D+00
9	2.81140D-11	-7.33929D-09	-1.70245D+00
10	-2.79488D-08	-3.86506D-10	3.85259D-09
11	-2.08246D-09	-6.67878D-11	2.00368D-10
12	8.69678D-09	1.68461D-10	-3.41445D-10
13	3.55457D-08	-4.27248D-11	-2.42044D-10
14	-1.59187D-01	4.58522D-10	4.47954D-10
15	-6.53757D+00	-1.97335D-10	-7.13403D-11
16	-2.97871D+00	2.31973D-10	-1.64102D-10
17	-1.27296D-09	4.07519D+00	-5.77115D-08
18	-3.17806D-11	2.52364D+00	-1.10893D-07
19	-4.20058D-10	-1.93886D+00	-1.11033D-07
20	-2.76844D-10	-4.03292D+00	1.19334D-07
21	-6.17560D-10	-1.62080D+00	-3.48437D-08
22	-5.06490D-10	1.23133D+00	1.07163D-07
23	-1.78922D-10	7.72822D-01	9.09720D-09
24	1.22999D-10	2.33679D-01	9.82105D-08

Table S27. The linear dipole moment surface of Pyridazine-d4. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol^{-1}}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	5.69930D-11	-1.70200D-08	-2.07130D+00
2	5.85779D-11	-3.22740D-08	6.21363D-01
3	-1.21598D-10	9.79181D-09	1.37911D+00
4	-1.41654D-10	5.82748D-08	4.06515D-01
5	-1.80246D-10	3.86965D-08	1.59227D+00
6	-1.54740D-10	3.12896D-08	1.64373D+00
7	2.13611D-10	2.42567D-08	-2.33855D+00
8	2.11296D-11	-1.17819D-08	-2.40213D+00
9	-1.44329D-11	-4.85334D-09	-1.40557D+00
10	-1.84088D-08	-3.76610D-10	1.73378D-09
11	1.31964D-09	-1.87218D-11	-7.15569D-12
12	4.92996D-09	1.05955D-11	-2.23595D-11
13	-3.32584D-08	2.10246D-11	-6.19108D-13
14	6.23999D-01	-3.27587D-10	-3.85106D-10
15	-4.20664D+00	1.71279D-11	1.48173D-10
16	-2.93426D+00	2.13723D-10	8.96445D-11
17	2.51486D-10	3.99119D+00	-3.09428D-08
18	-1.11944D-10	1.75869D+00	-7.81011D-08
19	-1.22553D-10	-9.15811D-01	-1.20017D-07
20	-8.01328D-11	-3.86624D+00	1.95184D-08
21	5.57255D-11	-1.32691D+00	-8.38474D-08
22	1.88501D-10	-9.43519D-02	3.65969D-08
23	2.11799D-10	2.73217D-01	-4.74961D-08
24	-2.87369D-10	1.38905D-01	9.86409D-08

Table S28. The linear dipole moment surface of Pyrazine. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol^{-1}}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	4.11647D-12	2.04772D-09	1.95939D-08
2	-1.78503D-11	-2.17065D-09	1.60687D-08
3	-9.36849D-12	-7.85933D-10	5.83305D-08
4	-5.21686D-12	-7.45725D-10	-3.73010D-09
5	-4.78204D-12	2.27962D-09	1.71112D-08
6	-4.61996D-09	2.53111D-11	-1.63396D-11
7	2.02744D-09	3.42335D-12	1.41698D-12
8	1.52683D-08	7.09790D-12	-8.49026D-10
9	-1.22583D-11	-1.40709D-08	1.50462D+00
10	-2.35082D-11	-1.93543D-09	-7.49527D-01
11	1.70003D-11	3.17020D-09	-2.36375D+00
12	8.17990D-11	3.10609D-10	-5.88700D+00
13	-5.29345D-09	-4.65323D-11	2.49018D-11
14	-3.81650D-09	-4.07016D-10	-1.98677D-11
15	5.29972D-12	7.91411D+00	-6.84609D-09
16	-9.12245D-12	-5.56157D+00	1.18625D-08
17	4.91111D-12	2.11278D+00	-2.18106D-08
18	-7.14315D-12	3.57414D+00	4.90681D-09
19	1.58597D-10	1.10911D-08	-4.91994D-08
20	-1.54899D-10	-8.08850D-09	3.55638D-08
21	-1.19276D-10	4.82807D-09	-2.94168D-08
22	-4.26986D-11	1.75933D-09	-2.73773D-08
23	-5.50888D+00	-2.90122D-12	-3.38918D-11
24	4.91941D+00	-7.08565D-13	-6.41237D-10

Table S29. The linear dipole moment surface of Pyrazine-d4. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol^{-1}}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	1.16942D-11	9.53560D-09	1.38800D-08
2	5.26202D-11	-2.15162D-09	3.25355D-08
3	8.29049D-12	5.05330D-09	-2.68132D-08
4	2.09698D-12	8.51258D-10	2.71023D-08
5	3.71588D-12	2.54963D-09	1.93715D-08
6	-4.52990D-09	-5.20610D-11	4.72560D-12
7	1.49997D-09	-3.30951D-14	7.37094D-12
8	2.36731D-08	-5.22277D-12	5.80070D-11
9	5.13338D-12	-9.18749D-09	1.50839D+00
10	-4.70364D-11	-3.46220D-09	1.65437D+00
11	-2.61205D-12	1.78596D-09	3.31813D+00
12	4.68001D-11	1.52783D-09	-4.40071D+00
13	-1.08340D-09	4.31066D-10	-8.92266D-11
14	4.52345D-09	1.33844D-10	2.63309D-12
15	1.50378D-12	7.04149D+00	-5.69292D-09
16	-3.52931D-11	-5.95506D+00	7.87991D-09
17	2.21779D-11	1.95736D+00	-2.14974D-08
18	8.32037D-12	1.16749D+00	6.41735D-09
19	7.04667D-10	8.59961D-09	-3.51160D-08
20	-1.84894D-10	-8.36450D-09	3.49478D-08
21	4.15420D-11	2.64887D-09	-1.81473D-07
22	9.33425D-11	1.73714D-09	-2.62171D-08
23	-2.54109D+00	-6.27594D-12	-5.16328D-11
24	-5.21162D+00	2.06748D-12	3.17256D-10

Table S30. The linear dipole moment surface of trans-butadiene. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol^{-1}}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	9.22103D-08	-3.32597D-07	3.78924D-10
2	-1.05521D-07	-1.61735D-07	1.04126D-09
3	8.57642D-08	-3.16577D-07	-1.03406D-09
4	-1.25335D-07	7.49660D-08	1.53685D-09
5	-4.91304D-08	3.74626D-07	3.62235D-10
6	-8.46888D-08	3.66031D-08	-7.66151D-10
7	-4.97262D-09	-7.69414D-08	-8.79643D-10
8	4.76458D-08	-1.94702D-08	1.15453D-09
9	-2.61479D-08	3.76156D-08	-1.93329D-09
10	5.51612D-11	-5.49738D-11	-5.87947D+00
11	-1.80683D-10	5.06938D-10	-9.31788D+00
12	-2.14096D-10	6.90315D-10	3.62218D+00
13	1.03248D-10	-1.56322D-10	8.27737D-01
14	5.76663D-10	7.47056D-10	-2.50646D-08
15	1.08559D-10	-4.92242D-10	6.88043D-08
16	1.16806D-09	2.10800D-09	-3.27060D-08
17	4.19724D+00	-2.10656D+00	3.97373D-10
18	-2.92780D+00	1.42526D+00	-1.60643D-10
19	4.00146D+00	1.64271D+00	-2.59822D-10
20	-1.61593D+00	-4.65056D+00	-2.78403D-12
21	-1.61600D+00	-8.88636D-01	2.31300D-10
22	-1.51340D+00	2.23462D-01	1.01741D-10
23	-1.43718D-01	-1.37694D+00	1.32192D-11
24	1.45506D-01	-1.68737D+00	1.34305D-10

Table S31. The linear dipole moment surface of trans-butadiene-d6. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol}^{-1}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	1.21773D-07	-2.77550D-07	5.11617D-10
2	8.24198D-10	-2.43841D-07	-6.70496D-10
3	9.10343D-08	-1.02772D-07	7.51419D-10
4	-1.34076D-07	2.52734D-08	5.62980D-10
5	-8.38588D-08	1.74927D-07	-6.58098D-10
6	3.29609D-09	2.17743D-07	-6.87305D-10
7	-2.41199D-08	4.21413D-08	7.29445D-10
8	2.84939D-08	9.50350D-09	-3.76433D-09
9	-2.66695D-08	4.48987D-08	-7.63478D-10
10	-5.01389D-12	-1.36171D-10	-2.29409D-01
11	1.02207D-10	-1.45185D-10	-8.23072D+00
12	-1.99942D-12	-3.70127D-10	2.80623D+00
13	-3.50198D-11	1.22359D-10	7.12360D-01
14	-1.48951D-10	-6.98010D-10	4.75251D-08
15	1.10044D-10	9.83605D-10	-4.34620D-08
16	6.25853D-10	1.64401D-09	-2.06639D-08
17	3.22641D+00	-1.01455D+00	2.81535D-11
18	-1.92917D+00	6.42680D-01	-1.27624D-10
19	2.93145D+00	3.18955D-01	-4.24307D-11
20	-7.27940D-01	-4.22300D+00	-5.44392D-10
21	-6.44324D-01	-8.28770D-01	1.16082D-10
22	1.76316D+00	1.33970D+00	-6.95698D-11
23	1.07481D-01	-1.20369D+00	1.78924D-10
24	1.36290D-01	-1.38705D+00	-8.72362D-11

Table S32. The linear dipole moment surface of Thiophene. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol^{-1}}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	-2.79827D-10	-2.70365D-07	1.11413D+00
2	-2.39083D-10	3.47997D-07	1.90453D+00
3	3.78796D-11	-7.92720D-08	-2.87452D+00
4	-4.50458D-11	-2.06948D-07	1.16694D+00
5	3.70506D-10	3.19490D-06	1.84978D+00
6	3.11381D-10	8.32679D-08	1.74960D+00
7	4.40244D-11	4.43077D-08	-4.82128D+00
8	-3.00012D-10	-3.91298D-08	4.52494D-01
9	1.59732D-08	-3.62703D-10	-2.10871D-09
10	4.32726D-08	-8.85157D-11	-1.24292D-09
11	-5.27517D-08	1.79047D-10	-1.68666D-09
12	-1.37080D-01	-8.29555D-10	-4.54454D-10
13	-1.15022D+01	4.49254D-10	-6.32244D-10
14	-7.55619D-01	-7.84236D-10	2.69899D-10
15	9.16806D-10	1.81462D-01	-3.09009D-07
16	-8.33356D-10	1.84446D+00	2.86861D-07
17	2.42800D-10	-4.04206D-01	-7.95300D-08
18	-3.24335D-10	3.28871D+00	2.71053D-07
19	2.07137D-09	2.00879D+00	-3.23038D-06
20	5.62445D-11	-1.13930D+00	-2.69159D-07
21	-1.72056D-10	6.87113D-01	4.92641D-08

Table S33. The linear dipole moment surface of Thiophene-d4. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The derivatives are in $\sqrt{km.mol^{-1}}$ unit.

Mode	$\frac{d\mu_x}{dq_i}$	$\frac{d\mu_y}{dq_i}$	$\frac{d\mu_z}{dq_i}$
1	-2.77794D-10	-1.17943D-07	1.04102D+00
2	-1.84035D-10	3.18551D-07	6.91252D-01
3	2.86926D-11	6.12500D-08	-3.24097D+00
4	7.86231D-11	-1.79410D-07	1.88924D+00
5	2.99032D-10	7.85575D-08	-1.05568D+00
6	2.80399D-10	-2.32259D-07	1.44359D+00
7	-1.05173D-10	-4.01925D-08	-4.05698D+00
8	5.17152D-10	5.40956D-08	-7.78683D-01
9	3.22071D-08	-4.43691D-10	-4.75167D-11
10	-3.14406D-08	-3.40278D-11	-9.66707D-10
11	-2.06912D-08	5.93678D-11	-1.82603D-09
12	5.00763D-01	-6.10208D-11	6.32432D-11
13	-8.55372D+00	1.46958D-10	-4.20670D-10
14	-5.14541D-01	7.47228D-10	-3.18995D-10
15	4.78820D-10	-4.68009D-02	-2.32424D-07
16	-6.31265D-10	1.27274D+00	2.69076D-07
17	1.69855D-11	-1.32041D+00	-1.13448D-07
18	3.80422D-10	-1.83238D+00	-9.20634D-08
18	-1.15372D-09	-2.02776D+00	-1.92780D-07
20	-7.85991D-10	2.34633D-01	2.10115D-07
21	-4.76898D-10	-1.15421D+00	-6.69075D-08

Table S34: The quartic potential energy surface of Pyrimidine. The calculation was done by using B3LYP/6-311++G(2d,2p) method using Gaussian 09 software. The force constants (F_i's) are in cm⁻¹ units.

I J	F _i (I,J)	I J K	F _i (I,J,K)	I J K L	F _i (I,J,K,L)	I J K L	F _i (I,J,K,L)
1 1	3201.75540	24 19 6	-8.95841	15 12 10 10	-112.86515	21 21 8 3	-0.43358
2 2	3171.67384	24 19 7	-18.24708	15 12 11 11	-19.96351	21 21 8 4	-6.70515
3 3	3155.55476	24 19 8	3.08533	15 12 12 12	6.21578	21 21 8 5	-11.50430
4 4	1607.14688	24 19 9	-8.03029	15 13 1 1	148.85698	21 21 8 6	-11.34349
5 5	1436.99400	24 20 1	-20.77786	15 13 2 2	-206.97229	21 21 8 7	2.47313
6 6	1162.76269	24 20 2	56.49583	15 13 3 3	-60.62118	21 21 8 8	4.55054
7 7	1082.71470	24 20 3	68.04453	15 13 4 4	5.43477	21 21 9 1	1.61774
8 8	1009.61930	24 20 4	-9.81736	15 13 5 5	4.65669	21 21 9 2	-2.58036
9 9	696.90072	24 20 5	2.33975	15 13 6 6	2.41359	21 21 9 3	-0.64566
10 10	1002.98792	24 20 6	-11.97915	15 13 7 7	2.26890	21 21 9 4	8.82901
11 11	409.16007	24 20 7	-11.43742	15 13 9 9	0.75818	21 21 9 5	-2.45789
12 12	1027.72101	24 20 8	1.17283	15 13 10 10	57.48839	21 21 9 6	10.74483
13 13	984.19117	24 20 9	4.73649	15 13 11 11	13.63966	21 21 9 7	3.66377
14 14	822.33769	24 21 1	-69.08109	15 13 12 12	61.56245	21 21 9 8	0.52203
15 15	737.70762	24 21 2	18.72861	15 13 13 12	89.59050	21 21 9 9	-0.31823
16 16	351.59394	24 21 3	-31.16022	15 13 13 13	58.38819	21 21 10 10	19.92164
17 17	3158.72801	24 21 4	-9.79910	15 14 1 1	-217.06900	21 21 11 10	-7.55763
18 18	1606.05303	24 21 5	-13.22655	15 14 2 2	-23.26627	21 21 11 11	-8.65143
19 19	1499.43396	24 21 6	16.16369	15 14 3 3	-103.83121	21 21 12 12	8.28294
20 20	1400.29392	24 21 7	12.99992	15 14 4 4	8.47767	21 21 13 12	-9.57056
21 21	1250.97416	24 21 8	-13.02284	15 14 5 5	9.08379	21 21 13 13	7.48085
22 22	1206.17663	24 21 9	6.81347	15 14 6 6	6.20857	21 21 14 12	-3.52449
23 23	1094.68642	24 22 1	6.27925	15 14 7 7	3.06997	21 21 14 13	-6.66984
24 24	637.74512	24 22 2	-30.23882	15 14 8 8	0.87789	21 21 14 14	13.46744
		24 22 3	2.33833	15 14 9 9	1.84763	21 21 15 12	-0.52867
		24 22 4	-26.38306	15 14 10 10	82.46685	21 21 15 13	1.98042
		24 22 5	-1.51411	15 14 11 11	15.84838	21 21 15 14	19.03213
		24 22 6	-11.74210	15 14 12 12	71.19657	21 21 15 15	4.55871
		24 22 7	1.13613	15 14 13 13	82.49196	21 21 16 12	10.37736
		24 22 8	3.98604	15 14 14 12	30.67329	21 21 16 13	0.28001
		24 22 9	-7.91355	15 14 14 13	-71.08457	21 21 16 14	4.45565
		24 23 1	94.95860	15 14 14 14	137.58298	21 21 16 15	-10.09546
		24 23 2	26.24605	15 15 1 1	-127.03355	21 21 16 16	-14.09737
		24 23 3	-20.49867	15 15 2 1	-0.40733	21 21 17 17	-85.88823
		24 23 4	-7.91962	15 15 2 2	-113.98171	21 21 18 17	0.35689
		24 23 5	23.18846	15 15 3 1	-0.68201	21 21 18 18	21.38839
		24 23 6	11.66684	15 15 3 2	1.83679	21 21 19 17	2.98487
		24 23 7	20.47738	15 15 3 3	-129.15506	21 21 19 18	2.65541
		24 23 8	5.25522	15 15 4 1	1.14085	21 21 19 19	13.95835
		24 23 9	5.52084	15 15 4 2	0.46573	21 21 20 17	-2.85370
		24 24 1	39.75736	15 15 4 3	3.84466	21 21 20 18	-5.64780
		24 24 2	-18.09488	15 15 4 4	-2.65225	21 21 20 19	-12.59204
		24 24 3	9.84076	15 15 5 1	-1.57235	21 21 20 20	20.90765
		24 24 4	18.49708	15 15 5 2	0.31511	21 21 21 17	3.23258
		24 24 5	5.76535	15 15 5 3	0.32745	21 21 21 18	-6.86244
		24 24 6	-7.10494	15 15 5 4	-7.88860	21 21 21 19	-6.80949
		24 24 7	-15.55378	15 15 5 5	0.21364	21 21 21 20	-9.46327
		24 24 9	-2.84753	15 15 6 1	1.31392	21 21 21 21	47.83528
				15 15 6 2	-1.01612	22 17 1 1	-0.51586
				15 15 6 3	-0.79545	22 17 2 2	-0.25785
				15 15 6 4	5.03863	22 17 3 3	-5.86937
				15 15 6 5	-6.70609	22 17 4 4	-0.29640
				15 15 6 6	-1.76193	22 17 5 5	5.39328
				15 15 7 1	-2.73099	22 17 6 6	2.74846
				15 15 7 2	0.72287	22 17 7 7	1.77381
				15 15 7 3	-1.78233	22 17 9 9	0.35347
				15 15 7 4	4.66629	22 17 10 10	6.17080
				15 15 7 5	-5.51697	22 17 11 11	1.25766
				15 15 7 6	4.14587	22 17 12 12	2.98049
				15 15 7 7	-2.13102	22 17 13 13	-0.37556
				15 15 8 1	0.56927	22 17 14 14	3.14881
				15 15 8 2	-0.19011	22 17 15 15	3.60703
				15 15 8 3	-0.10261	22 17 16 16	-1.20360
				15 15 8 4	-0.23160	22 17 17 17	-6.50775
				15 15 8 5	0.61316	22 18 1 1	5.72530
				15 15 8 6	0.21628	22 18 2 2	41.90310
				15 15 8 7	0.54319	22 18 3 3	7.69136
				15 15 8 8	-3.85867	22 18 4 4	8.35981
				15 15 9 1	0.88525	22 18 5 5	-5.52492
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				15 15 9 5	-5.09418	22 18 9 9	-3.25294
				15 15 9 6	3.25907	22 18 10 10	-0.27552
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				15 15 11 10	-44.98501	22 18 14 14	-0.30334
				15 15 11 11	26.78747	22 18 15 15	-2.54016
				15 15 12 12	90.84772	22 18 16 16	-8.82683
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I	J	K	F(I,J,K)	I	J	K	L	F(I,J,K,L)	I	J	K	L	F(I,J,K,L)	I	J	K	L	F(I,J,K,L)
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9	8	4	-28.46321	7	5	1	1	3.99348	16	16	8	1	-0.89817	22	22	7	7	3.19675
9	8	5	-19.71445	7	5	2	2	0.64615	16	16	8	4	7.58992	22	22	8	1	-0.80775
9	8	6	-6.08725	7	5	3	3	52.53906	16	16	8	5	4.98053	22	22	8	2	1.04457
9	8	8	2.54913	7	5	4	4	-2.72936	16	16	8	6	1.81253	22	22	8	3	-2.28212
9	9	1	3.76132	7	5	5	1	0.36607	16	16	8	7	-2.16311	22	22	8	4	13.95769
9	9	2	-5.73652	7	5	5	2	-0.58461	16	16	8	8	-9.84839	22	22	8	5	7.66087
9	9	3	20.39287	7	5	5	3	1.09063	16	16	9	1	-0.41203	22	22	8	6	-10.72578
9	9	4	-9.30985	7	5	5	4	5.98833	16	16	9	2	1.26234	22	22	8	7	13.48787
9	9	5	2.96972	7	5	5	5	-6.81956	16	16	9	3	1.21911	22	22	8	8	12.06492
9	9	6	10.28290	7	6	1	1	-2.86054	16	16	9	4	0.61370	22	22	9	1	0.93473
9	9	7	1.62278	7	6	2	2	-0.05468	16	16	9	5	-4.68989	22	22	9	2	-0.38000
9	9	8	-22.55319	7	6	3	3	-38.52979	16	16	9	6	1.06075	22	22	9	3	-1.71606
9	9	9	3.80799	7	6	4	4	4.92486	16	16	9	7	3.14832	22	22	9	4	9.40406
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10	10	2	-58.28203	7	6	6	1	-0.05778	16	16	9	9	1.52198	22	22	9	6	1.25857
10	10	3	478.27966	7	6	6	2	-0.57511	16	16	10	10	49.19125	22	22	9	7	-1.51694
10	10	4	-7.43370	7	6	6	3	-0.56253	16	16	11	10	-19.00411	22	22	9	8	-1.40810
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10	10	6	9.35362	7	6	6	5	-1.78908	16	16	12	12	65.61207	22	22	10	10	-5.77938
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11	11	6	-46.81264	7	7	6	2	0.16296	17	17	3	1	133.64852	22	22	17	17	-5.59609
11	11	7	33.15818	7	7	6	3	-0.14913	17	17	3	2	-61.86488	22	22	18	17	-0.58734
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12	12	3	157.74075	7	7	7	2	-0.33866	17	17	4	4	-72.60704	22	22	20	17	2.14799
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12	12	9	-0.55494	8	1	1	1	11.41795	17	17	6	1	-2.16348	22	22	21	19	-1.90190
13	12	1	-157.68394	8	2	1	1	0.95668	17	17	6	2	0.41482	22	22	21	20	3.88286
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13	12	9	1.64830	8	4	1	1	0.56957	17	17	7	4	-50.56633	23	17	1	1	2.19038
13	13	1	249.78998	8	4	2	2	0.26867	17	17	7	5	57.26670	23	17	2	2	0.19847
13	13	2	-392.74645	8	4	3	3	-0.26187	17	17	7	6	-41.85744	23	17	3	3	-0.35025
13	13	3	-54.77134	8	4	4	1	0.89743	17	17	7	7	-36.62698	23	17	4	4	-1.04994
13	13	4	20.08092	8	4	4	2	0.40856	17	17	8	1	0.80209	23	17	5	5	-2.56054
13	13	5	12.38039	8	4	4	3	-1.09663	17	17	8	2	-0.26150	23	17	6	6	-0.32744
13	13	6	4.03745	8	4	4	4	13.13908	17	17	8	3	3.15767	23	17	7	7	-0.72556
13	13	7	-9.82667	8	5	2	2	1.13471	17	17	8	4	-0.33018	23	17	8	8	0.44751
13	13	8	-5.20179	8	5	3	3	-1.17015	17	17	8	5	-1.37255	23	17	9	9	-0.34932
13	13	9	-2.70917	8	5	4	4	9.17788	17	17	8	6	0.34775	23	17	10	10	-2.82825
14	12	1	165.08727	8	5	5	1	-0.20080	17	17	8	7	1.10791	23	17	12	12	-2.07362
14	12	2	3.20884	8	5	5	2	0.38740	17	17	8	8	-0.83624	23	17	13	13	-0.99985
14	12	3	-210.78877	8	5	5	3	-0.63255	17	17	9	1	-0.95955	23	17	14	14	0.15311
14	12	4	9.29084	8	5	5	4	2.22117	17	17	9	2	0.17172	23	17	15	15	0.46848
14	12	5	2.50594	8	5	5	5	-3.06801	17	17	9	3	-2.47156	23	17	16	16	-0.50847
14	12	6	-10.95677	8	6	1	1	-0.62500	17	17	9	4	-29.48591	23	17	17	17	-0.51190
14	12	8	-6.86196	8	6	2	2	0.28361	17	17	9	5	35.04865	23	18	1	1	114.92287
14	12	9	-7.54548	8	6	3	3	0.28753	17	17	9	6	-25.80869	23	18	2	2	-27.30059
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14	13	3	152.73156	8	6	6	1	0.30606	17	17	9	9	-13.86248	23	18	5	5	-6.20729
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I	J	K	FI(I,J,K)	I	J	K	L	FI(I,J,K,L)	I	J	K	L	FI(I,J,K,L)	I	J	K	L	FI(I,J,K,L)
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14	14	7	2.18850	8	7	5	5	0.26439	17	17	15	12	142.67130	23	18	15	15	-5.76711
14	14	8	10.23540	8	7	6	6	0.28164	17	17	15	13	-72.73204	23	18	16	16	-4.03562
14	14	9	0.91739	8	7	7	1	-1.32224	17	17	15	14	-97.14064	23	18	17	17	3.42635
15	12	1	65.99779	8	7	7	3	-1.18194	17	17	15	15	-129.52176	23	18	18	17	0.13675
15	12	2	-136.67785	8	7	7	4	-4.99114	17	17	16	12	-95.29757	23	18	18	18	1.32463
15	12	3	-257.55929	8	7	7	5	0.59096	17	17	16	13	48.85926	23	19	1	1	-161.35268
15	12	4	9.23890	8	7	7	6	1.22910	17	17	16	14	65.26026	23	19	2	2	-53.85729
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15	12	8	-3.20626	8	8	2	2	-1.08543	18	17	1	1	-2.09607	23	19	6	6	-4.04430
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15	13	1	-133.78156	8	8	3	2	-0.11994	18	17	3	3	-10.66185	23	19	8	8	-3.06525
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16	13	7	16.95293	9	4	4	2	-0.36969	18	18	7	7	11.54592	23	21	6	6	4.52743
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16	13	9	8.73640	9	4	4	4	13.55420	18	18	8	2	0.51647	23	21	8	8	0.33539
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17 15 10	321.46274	9 8 2 2	0.23634	18 18 17 17	-19.46655	23 22 17 17	-1.04326
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19 19 1	108.75062	10 10 15 1	16.19492	19 19 32 1	0.67569	23 23 10 14	10.60375
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19 19 7	-53.12323	10 10 21 1	0.76886	19 19 38 1	1.56979	23 23 10 20	0.11535
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20	17	6	-84.47750	10	10	9	4	9.34366	19	19	14	14	12.85390	23	23	22	22	17.09197
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20	17	8	1.53986	10	10	9	6	6.98161	19	19	15	13	4.45292	23	23	23	18	-33.35370
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20	18	3	-75.13590	10	10	10	10	267.38751	19	19	16	13	4.76226	23	23	23	22	1.71056
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23 14 10	-13.19466	13 13 8 8	-2.17734	21 17 10 10	4.34785	24 23 19 19	7.06575
23 14 11	-27.13635	13 13 9 1	1.56224	21 17 11 11	2.80675	24 23 20 20	-0.41522
23 15 10	-6.24783	13 13 9 2	1.94116	21 17 12 12	3.25312	24 23 21 21	14.62918
23 15 11	18.52643	13 13 9 3	-0.28662	21 17 13 13	0.26449	24 23 22 22	-4.78192
23 16 10	-9.51665	13 13 9 4	1.00277	21 17 14 14	-0.34435	24 23 23 18	-18.66331
23 16 11	-11.24915	13 13 9 5	-1.58605	21 17 15 15	2.61688	24 23 23 19	17.63381
23 17 1	2.33967	13 13 9 6	1.17456	21 17 16 16	-1.83468	24 23 23 20	-8.65110
23 17 3	-2.26047	13 13 9 7	0.37591	21 17 17 17	-14.64827	24 23 23 21	-18.34277
23 17 4	-2.86228	13 13 9 8	0.48582	21 18 1 1	-67.64336	24 23 23 22	3.35179
23 17 5	10.28720	13 13 9 9	-1.57132	21 18 2 2	-27.64202	24 23 23 23	30.52654
23 17 6	-10.47878	13 13 10 10	32.59813	21 18 3 3	-40.54380	24 24 1 1	-29.92211
23 17 7	-8.45150	13 13 11 10	-13.96830	21 18 4 4	4.59783	24 24 2 1	-1.25999
23 17 8	-5.04856	13 13 11 11	7.15372	21 18 5 5	-4.49565	24 24 2 2	-17.64161
23 17 9	-10.07647	13 13 12 12	145.86252	21 18 6 6	-3.03178	24 24 3 1	4.97427
23 18 1	-99.05276	13 13 13 13	83.27400	21 18 7 7	5.61501	24 24 3 2	-0.32721
23 18 2	-28.59339	13 13 13 13	239.98154	21 18 8 8	-3.08880	24 24 3 3	-13.17155
23 18 3	19.53153	14 12 1 1	-177.91395	21 18 9 9	3.16450	24 24 4 1	0.10333
23 18 4	46.29621	14 12 2 2	-29.85048	21 18 10 10	9.77965	24 24 4 3	0.94030
23 18 5	-49.57921	14 12 3 3	86.33196	21 18 11 11	2.67566	24 24 4 4	-8.51611
23 18 6	-64.36660	14 12 4 4	-2.88523	21 18 12 12	11.59422	24 24 5 1	-0.66873

I J K	FI(I,J,K)	I J K L	FI(I,J,K,L)	I J K L	FI(I,J,K,L)	I J K L	FI(I,J,K,L)
23 18 7	-46.02108	14 12 5 5	-7.55543	21 18 13 13	11.93349	24 24 5 2	0.48229
23 18 8	-10.65242	14 12 6 6	-5.23041	21 18 14 14	14.29859	24 24 5 3	-0.52119
23 18 9	-3.40359	14 12 7 7	-1.52004	21 18 15 15	9.99114	24 24 5 4	-6.13451
23 19 1	141.69933	14 12 9 9	-0.96788	21 18 16 16	11.59620	24 24 5 5	-0.36951
23 19 2	-30.52730	14 12 10 10	-85.24993	21 18 17 17	-38.84244	24 24 6 1	0.55441
23 19 3	-45.69302	14 12 11 11	-15.21338	21 18 18 17	0.41166	24 24 6 2	0.36241
23 19 4	43.16743	14 12 12 12	-4.57175	21 18 18 18	-3.48045	24 24 6 3	0.14834
23 19 5	18.56462	14 13 1 1	272.52788	21 19 1 1	87.63594	24 24 6 4	4.39121
23 19 6	-14.98651	14 13 2 2	-38.53429	21 19 2 2	-52.00951	24 24 6 5	-1.47908
23 19 7	30.99265	14 13 3 3	-33.41788	21 19 3 3	-43.49142	24 24 6 6	-0.16013
23 19 8	34.81104	14 13 4 4	0.44799	21 19 4 4	4.80663	24 24 7 1	-0.90823
23 19 9	-5.53850	14 13 5 5	1.58675	21 19 5 5	1.99273	24 24 7 3	0.10803
23 20 1	-71.14174	14 13 6 6	1.39337	21 19 6 6	-0.13375	24 24 7 4	0.72215
23 20 2	-62.27245	14 13 7 7	0.38493	21 19 7 7	3.22860	24 24 7 5	-1.82552
23 20 3	21.57414	14 13 8 8	-1.36736	21 19 8 8	-0.58378	24 24 7 6	3.22932
23 20 4	-18.61770	14 13 9 9	0.94688	21 19 9 9	4.05189	24 24 7 7	1.30871
23 20 5	30.83195	14 13 10 10	43.02431	21 19 10 10	11.97730	24 24 8 1	0.53609
23 20 6	16.12478	14 13 11 11	10.39429	21 19 11 11	4.77656	24 24 8 2	-0.14919
23 20 7	-6.54345	14 13 12 12	-6.49481	21 19 12 12	6.38174	24 24 8 3	-0.46606
23 20 8	6.15819	14 13 13 12	57.11514	21 19 13 13	1.03097	24 24 8 4	-3.25441
23 20 9	-1.79593	14 13 13 13	-53.94995	21 19 14 14	-8.57960	24 24 8 5	-1.08173
23 21 1	-134.47405	14 14 1 1	-383.73052	21 19 15 15	1.53777	24 24 8 6	0.23016
23 21 2	-28.77051	14 14 2 1	-27.29072	21 19 16 16	3.32194	24 24 8 7	1.90264
23 21 3	21.76448	14 14 2 2	-8.00411	21 19 17 17	-52.60191	24 24 8 8	-3.95279
23 21 4	30.86311	14 14 3 1	79.00440	21 19 18 18	-5.15160	24 24 9 1	0.30159
23 21 5	31.31859	14 14 3 2	15.32071	21 19 19 17	2.15639	24 24 9 2	0.18752
23 21 6	58.93957	14 14 3 3	-93.22098	21 19 19 18	10.81078	24 24 9 4	1.73645
23 21 7	-5.47454	14 14 4 1	3.60388	21 19 19 19	-0.44721	24 24 9 5	-1.99056
23 21 8	-16.60870	14 14 4 2	0.22276	21 20 1 1	-42.37466	24 24 9 6	0.67519
23 21 9	13.04952	14 14 4 3	0.83717	21 20 2 2	-63.36049	24 24 9 9	1.05406
23 22 1	13.68440	14 14 4 4	-5.66103	21 20 3 3	84.16178	24 24 10 10	1.56451
23 22 2	25.43947	14 14 5 1	-5.69164	21 20 4 4	-10.32973	24 24 11 10	-1.03104
23 22 3	7.23305	14 14 5 2	-0.45103	21 20 5 5	-14.94519	24 24 11 11	4.58734
23 22 4	147.88882	14 14 5 3	3.39399	21 20 6 6	-7.28088	24 24 12 12	1.87727
23 22 5	67.91540	14 14 5 4	-7.58214	21 20 7 7	-6.50930	24 24 13 12	-1.01512
23 22 6	-39.16090	14 14 5 5	0.91439	21 20 8 8	0.95167	24 24 13 13	4.77172
23 22 7	-36.15557	14 14 6 1	0.48024	21 20 9 9	-3.83219	24 24 14 12	1.19960
23 22 8	-0.84262	14 14 6 2	0.74931	21 20 10 10	-22.96158	24 24 14 13	-2.99210
23 22 9	13.83345	14 14 6 3	-1.99081	21 20 11 11	-0.30200	24 24 14 14	6.30314
23 23 1	249.50457	14 14 6 4	5.43999	21 20 12 12	-4.27660	24 24 15 12	1.14985
23 23 2	-1.46717	14 14 6 5	-5.36085	21 20 13 13	8.03662	24 24 15 13	-0.51993
23 23 3	-63.28581	14 14 6 6	0.26034	21 20 14 14	0.28888	24 24 15 14	5.06814
23 23 4	6.66402	14 14 7 1	-6.50571	21 20 15 15	-2.84059	24 24 15 15	1.94963
23 23 5	-8.55003	14 14 7 2	-0.49937	21 20 16 16	-4.37703	24 24 16 12	0.90927
23 23 6	-7.81739	14 14 7 3	0.90131	21 20 17 17	95.80641	24 24 16 13	-0.59753
23 23 7	-40.22062	14 14 7 4	2.43266	21 20 18 18	3.75387	24 24 16 14	-1.86881
23 23 8	-60.80055	14 14 7 5	-4.90353	21 20 19 19	6.58092	24 24 16 15	-0.37405
23 23 9	-38.46164	14 14 7 6	3.86382	21 20 20 17	2.20295	24 24 16 16	-3.01146
24 12 10	-4.34878	14 14 7 7	1.02212	21 20 20 18	14.51881	24 24 17 17	-11.73679
24 12 11	5.59644	14 14 8 1	-1.36203	21 20 20 19	14.60601	24 24 18 17	1.00675
24 13 10	8.07969	14 14 8 3	-0.54303	21 20 20 20	-6.83847	24 24 18 18	1.26359
24 13 11	5.03521	14 14 8 4	-1.16773	21 21 1 1	-84.56813	24 24 19 17	0.54398
24 14 11	7.26275	14 14 8 7	0.20133	21 21 2 1	-2.74489	24 24 19 18	-3.29288
24 15 10	-4.45629	14 14 8 8	-3.43130	21 21 2 2	-22.75616	24 24 19 19	4.62292
24 15 11	7.16152	14 14 9 1	1.49863	21 21 3 1	-0.40484	24 24 20 17	-0.80791
24 16 10	-5.61766	14 14 9 2	0.43571	21 21 3 2	8.43700	24 24 20 18	1.92127
24 16 11	12.90649	14 14 9 3	-0.90004	21 21 3 3	-84.96656	24 24 20 20	7.79504
24 17 1	0.79809	14 14 9 4	1.77371	21 21 4 1	0.77291	24 24 21 17	0.46544
24 17 2	-0.27194	14 14 9 5	-3.41589	21 21 4 2	-0.44577	24 24 21 18	7.40501
24 17 3	4.45913	14 14 9 6	0.98239	21 21 4 3	6.25461	24 24 21 19	-0.88262
24 17 4	-44.76891	14 14 9 7	1.98129	21 21 4 4	10.97768	24 24 21 20	0.43415
24 17 5	51.93038	14 14 9 8	-1.01298	21 21 5 1	-0.82467	24 24 21 21	4.92503
24 17 6	-37.83606	14 14 9 9	-1.55703	21 21 5 3	-0.88634	24 24 22 17	0.38510
24 17 7	-24.96214	14 14 10 10	63.62373	21 21 5 4	-5.59262	24 24 22 18	-0.59382
24 17 8	-1.02747	14 14 11 10	-24.73655	21 21 5 5	30.45509	24 24 22 19	-5.50623
24 17 9	-20.17387	14 14 11 11	17.00969	21 21 6 1	0.75110	24 24 22 20	-1.17728
24 18 1	-56.06747	14 14 12 12	76.58116	21 21 6 2	0.28110	24 24 22 21	-3.99972
24 18 2	31.62846	14 14 13 12	-84.26186	21 21 6 3	0.95966	24 24 22 22	-9.62878
24 18 3	-11.89400	14 14 13 13	114.69865	21 21 6 4	13.28515	24 24 23 18	-2.90254
24 18 4	-3.42725	14 14 14 12	78.87296	21 21 6 5	1.54043	24 24 23 19	10.73083
24 18 5	11.03008	14 14 14 13	-137.70371	21 21 6 6	20.93071	24 24 23 20	-2.11762
24 18 6	11.98642	14 14 14 14	216.96655	21 21 7 1	-1.09382	24 24 23 21	-8.72438
24 18 7	19.96433	15 12 1 1	-94.15656	21 21 7 2	-1.23207	24 24 23 22	3.00059
24 18 8	22.50406	15 12 2 2	-156.18831	21 21 7 3	2.84216	24 24 23 23	11.48252
24 18 9	-18.74006	15 12 3 3	121.97354	21 21 7 4	8.49279	24 24 24 17	-0.21361
24 19 1	54.07641	15 12 4 4	-8.36369	21 21 7 5	-9.62481	24 24 24 18	-4.91847
24 19 2	62.76480	15 12 5 5	-7.23215	21 21 7 6	9.67684	24 24 24 20	-1.32280
24 19 3	-33.16179	15 12 6 6	-5.43967	21 21 7 7	6.70365	24 24 24 21	-4.65211
24 19 4	11.47054	15 12 7 7	-4.18166	21 21 8 1	0.24314	24 24 24 23	5.79726
24 19 5	-25.53903	15 12 9 9	-1.36489	21 21 8 2	2.42088	24 24 24 24	7.64070

Table S35: The quartic potential energy surface of Pyrimidine-d4. The calculation was done by using B3LYP/6-311++G(2d,2p) method. The force constants (F) are in cm^{-1} units.

I J	F(I,J)	I J K	F(I,J,K)	I J K L	F(I,J,K,L)	I J K L	F(I,J,K,L)
1 1	2373.20410	24 18 5	12.74289	15 12 5 5	3.92871	21 21 8 4	-5.48338
2 2	2347.31359	24 18 6	-2.00956	15 12 6 6	0.23449	21 21 8 5	6.30456
3 3	2328.87749	24 18 7	21.51349	15 12 7 7	0.61147	21 21 8 6	-2.99552
4 4	1571.23541	24 18 8	-11.12271	15 12 8 8	11.09711	21 21 8 7	0.59168
5 5	1305.52324	24 18 9	-16.80931	15 12 9 9	2.06939	21 21 8 8	13.58167
6 6	1066.99001	24 19 1	-35.02691	15 12 10 10	52.79998	21 21 9 1	0.39641
7 7	993.65962	24 19 2	-36.97245	15 12 11 11	20.82111	21 21 9 2	0.59466
8 8	884.35864	24 19 3	12.43470	15 12 12 12	9.80024	21 21 9 4	2.17222
9 9	674.14544	24 19 4	-4.89780	15 13 1 1	13.05866	21 21 9 5	-4.05172
10 10	813.87986	24 19 5	31.73642	15 13 2 2	118.90871	21 21 9 6	0.99028
11 11	376.16410	24 19 6	-9.98319	15 13 3 3	-20.69105	21 21 9 8	-6.69168
12 12	868.24817	24 19 7	-4.31979	15 13 4 4	0.71820	21 21 9 9	2.93362
13 13	850.41351	24 19 8	-14.80370	15 13 5 5	0.40773	21 21 10 10	8.20536
14 14	674.94114	24 19 9	12.92079	15 13 6 6	0.17504	21 21 11 10	-6.01062
15 15	562.64216	24 20 1	-25.18237	15 13 8 8	5.04683	21 21 11 11	-2.66934
16 16	302.94635	24 20 2	-11.98245	15 13 9 9	1.33378	21 21 12 12	3.68886
17 17	2336.64354	24 20 3	-16.47291	15 13 10 10	30.60689	21 21 13 12	0.21536
18 18	1570.24879	24 20 4	-22.73130	15 13 11 11	9.00155	21 21 13 13	11.72573
19 19	1358.09972	24 20 5	-4.85390	15 13 12 12	7.24837	21 21 14 12	-2.66950
20 20	1215.81696	24 20 6	-6.00831	15 13 13 12	13.99780	21 21 14 13	5.84027
21 21	1054.06349	24 20 7	-2.29910	15 13 13 13	-53.30704	21 21 14 14	4.88360
22 22	936.46445	24 20 9	-3.18976	15 14 1 1	-136.10522	21 21 15 12	6.05784
23 23	832.92924	24 21 1	-19.79536	15 14 2 2	58.24597	21 21 15 13	-5.75253
24 24	618.42285	24 21 2	26.08878	15 14 3 3	-12.19605	21 21 15 14	-0.46562
		24 21 3	67.07729	15 14 4 4	0.68186	21 21 15 15	12.44434
I J K	F(I,J,K)	24 21 4	-8.28893	15 14 5 5	1.18913	21 21 16 12	-2.36698
		24 21 5	-5.54321	15 14 6 6	1.42017	21 21 16 13	-10.53206
1 1 1	-974.03713	24 21 6	0.70871	15 14 8 8	1.72275	21 21 16 14	-1.95639
2 1 1	-178.80410	24 21 7	0.67670	15 14 10 10	4.93955	21 21 16 15	0.88556
2 2 1	-187.25124	24 21 8	11.57807	15 14 12 12	21.77623	21 21 16 16	2.07753
2 2 2	1008.25542	24 21 9	1.77272	15 14 13 13	-29.03436	21 21 17 17	-51.50295
3 1 1	240.16055	24 22 1	-22.09689	15 14 14 12	-41.78026	21 21 18 17	2.15836
3 2 1	124.36523	24 22 2	50.84268	15 14 14 13	-29.18794	21 21 18 18	1.36396
3 2 2	325.47161	24 22 3	-22.43508	15 14 14 14	83.78850	21 21 19 17	1.08365
3 3 1	-400.45458	24 22 4	2.55309	15 15 1 1	-111.00418	21 21 19 18	-1.61218
3 3 2	283.12878	24 22 5	2.19350	15 15 2 1	0.48109	21 21 19 19	3.88410
3 3 3	-501.64515	24 22 6	7.49619	15 15 2 2	-99.29810	21 21 20 17	2.17090
4 1 1	73.57214	24 22 7	-5.53516	15 15 3 1	-5.70030	21 21 20 18	0.19671
4 2 1	11.13716	24 22 8	-15.36250	15 15 3 2	7.96220	21 21 20 19	1.30155
4 2 2	22.96260	24 22 9	4.67311	15 15 3 3	-121.63267	21 21 20 20	0.63390
4 3 1	-14.40765	24 23 1	97.19501	15 15 4 1	6.28766	21 21 21 17	0.33817
4 3 3	20.28187	24 23 2	37.22372	15 15 4 2	-0.37765	21 21 21 18	2.46359
4 4 1	16.45579	24 23 3	-18.31534	15 15 4 3	-0.87310	21 21 21 19	-2.72813
4 4 2	-15.25851	24 23 4	-4.07281	15 15 4 4	-1.53292	21 21 21 20	-9.08372
4 4 3	52.02130	24 23 5	19.84025	15 15 5 1	7.02320	21 21 21 21	22.65987
4 4 4	-172.33460	24 23 6	-6.93291	15 15 5 2	-4.21017	22 17 1 1	-2.80045
5 1 1	-77.07092	24 23 7	9.10318	15 15 5 3	-3.66421	22 17 2 2	-0.36583
5 2 1	-16.81623	24 23 9	1.32241	15 15 5 4	-2.19703	22 17 3 3	-7.60316
5 2 2	49.29613	24 24 1	58.14202	15 15 5 5	-1.24542	22 17 4 4	2.23936
5 3 1	3.67781	24 24 2	-14.55348	15 15 6 1	5.42172	22 17 5 5	0.78660
5 3 2	33.66250	24 24 4	18.00123	15 15 6 2	-6.33221	22 17 6 6	0.08437
5 3 3	-32.42946	24 24 6	2.31238	15 15 6 3	4.47072	22 17 7 7	0.43319
5 4 1	-19.04570	24 24 7	2.96881	15 15 6 5	-0.70790	22 17 8 8	0.18227
5 4 2	9.95611	24 24 8	11.28905	15 15 6 6	-4.78479	22 17 9 9	0.36261
5 4 3	-33.74779	24 24 9	-2.32103	15 15 7 1	-4.80714	22 17 10 10	1.81476
5 4 4	-43.59195			15 15 7 2	0.68261	22 17 11 11	1.74293
5 5 1	18.29611	I J K L	F(I,J,K,L)	15 15 7 6	-1.33159	22 17 12 12	0.93424
5 5 2	-12.92776	1 1 1 1	412.38193	15 15 7 7	-2.38770	22 17 13 13	0.26486
5 5 3	25.30860	2 1 1 1	93.08885	15 15 8 1	2.59236	22 17 14 14	-0.70524
5 5 4	76.93133	2 2 1 1	32.15508	15 15 8 2	0.20013	22 17 15 15	2.08233
5 5 5	47.71333	2 2 2 1	-44.97714	15 15 8 3	3.27736	22 17 17 17	-11.40406
6 1 1	27.38755	2 2 2 2	451.00248	15 15 8 4	-4.70714	22 18 1 1	-3.00203
6 2 1	-10.10121	3 1 1 1	-136.79856	15 15 8 5	6.54175	22 18 2 2	-28.67610
6 2 2	68.71624	3 2 1 1	-44.59406	15 15 8 6	-3.12681	22 18 3 3	-14.77723
6 3 1	14.49501	3 2 2 1	-18.78374	15 15 8 7	0.31908	22 18 4 4	-3.37065
6 3 2	6.07579	3 2 2 2	153.65461	15 15 8 8	11.71312	22 18 5 5	-4.95450
6 3 3	58.25582	3 3 1 1	89.60026	15 15 9 1	-0.61629	22 18 6 6	-1.10600
6 4 1	14.32911	3 3 2 1	-16.49426	15 15 9 2	1.31332	22 18 7 7	-0.79412
6 4 2	4.40499	3 3 2 2	78.33080	15 15 9 3	1.79739	22 18 8 8	3.68192
6 4 3	5.05724	3 3 3 1	53.54418	15 15 9 4	4.31052	22 18 9 9	2.26677
6 4 4	93.33962	3 3 3 2	-38.83102	15 15 9 5	-3.51383	22 18 10 10	2.63201
6 5 1	-10.98530	4 1 1 1	192.14355	15 15 9 6	0.82208	22 18 11 11	1.29577
6 5 2	3.39212	4 2 1 1	-31.48964	15 15 9 8	-8.74018	22 18 12 12	2.29233
6 5 3	-1.24568	4 2 2 1	-7.06106	15 15 9 9	2.32148	22 18 13 13	6.27942
6 5 4	-10.86827	4 2 2 2	-3.21838	15 15 10 10	85.45121	22 18 14 14	1.38862
6 5 5	48.06731	4 2 2 3	11.76592	15 15 11 10	-49.50325	22 18 15 15	3.57523
6 6 1	1.15150	4 3 1 1	10.77348	15 15 11 11	35.29114	22 18 16 16	7.41208
6 6 2	3.13843	4 3 2 1	5.00481	15 15 12 12	45.48652	22 18 17 17	-14.32995
6 6 3	0.96261	4 3 2 2	-5.60353	15 15 12 13	15.70224	22 18 18 17	0.82052
6 6 4	-5.55016	4 3 3 1	0.76731	15 15 13 13	52.93292	22 18 18 18	-6.79901
6 6 6	43.37251	4 3 3 2	1.43992	15 15 14 12	-32.99408	22 19 1 1	2.25681
7 1 1	-58.54608	4 3 3 3	-1.41172	15 15 14 13	15.21399	22 19 2 2	42.47719
7 2 1	-8.12309	4 4 1 1	1.76582	15 15 14 14	76.28385	22 19 3 3	19.70687
7 2 2	-17.91799	4 4 2 1	-1.97593	15 15 15 12	33.47450	22 19 4 4	9.50482
7 3 1	11.31480	4 4 2 2	-4.96249	15 15 15 13	-8.90958	22 19 5 5	1.11589
7 3 2	3.41092	4 4 3 1		15 15 15 14	31.82956	22 19 6 6	0.30858

I	J	K	Fl(I,J,K)	I	J	K	L	Fl(I,J,,K,L)	I	J	K	L	Fl(I,J,K,L)	I	J	K	L	Fl(I,J,K,L)
7	3	3	-20.16025	4	4	3	2	3.09101	15	15	15	15	124.59309	22	19	7	7	2.14490
7	4	1	-3.00705	4	4	3	3	-11.81578	16	12	1	1	47.75628	22	19	8	8	-4.60357
7	4	2	5.81843	4	4	4	1	-2.20517	16	12	2	2	-10.81822	22	19	9	9	-1.23046
7	4	3	3.95737	4	4	4	2	2.00805	16	12	3	3	40.67881	22	19	10	10	-3.97577
7	4	4	-146.42917	4	4	4	3	-1.97709	16	12	4	4	-4.34742	22	19	11	11	-6.58448
7	5	1	5.86922	4	4	4	4	37.52831	16	12	5	5	-2.27435	22	19	12	12	-2.68026
7	5	2	9.65839	5	1	1	1	30.48262	16	12	7	7	-0.77919	22	19	13	13	-6.81658
7	5	3	12.94970	5	2	1	1	6.66737	16	12	8	8	-8.60634	22	19	14	14	-2.86128
7	5	4	-31.99542	5	2	2	1	-0.89884	16	12	10	10	-30.58716	22	19	15	15	-4.50408
7	5	5	-97.07535	5	2	2	2	29.12604	16	12	11	11	-14.12530	22	19	16	16	-2.40157
7	6	1	-9.06663	5	3	1	1	-8.19447	16	12	12	12	-13.25255	22	19	17	17	18.34236
7	6	2	5.19496	5	3	2	2	10.77789	16	13	1	1	17.14368	22	19	18	18	-1.34022
7	6	3	-3.14888	5	3	3	1	9.06180	16	13	2	2	116.80148	22	19	19	19	-0.50328
7	6	4	9.74024	5	3	3	2	1.75386	16	13	3	3	38.39637	22	19	19	18	-1.40868
7	6	5	-5.21772	5	3	3	3	10.04255	16	13	4	4	-2.57966	22	19	19	19	3.38978
7	6	6	-24.99419	5	4	1	1	0.80426	16	13	5	5	-7.32851	22	20	1	1	-2.79652
7	7	1	6.96965	5	4	2	2	0.56234	16	13	7	7	-2.49046	22	20	2	2	21.57281
7	7	2	-8.78046	5	4	3	3	12.36898	16	13	8	8	-3.49701	22	20	3	3	-11.96142
7	7	3	4.91419	5	4	4	1	0.30099	16	13	9	9	-0.57098	22	20	4	4	-10.39325
7	7	4	-5.81319	5	4	4	2	1.57316	16	13	10	10	-18.49101	22	20	5	5	7.96655
7	7	5	8.54744	5	4	4	3	-1.28185	16	13	11	11	-5.11545	22	20	6	6	0.15798
7	7	6	33.36012	5	4	4	4	4.73087	16	13	12	12	-6.94625	22	20	7	7	-1.06505
7	7	7	-83.38854	5	5	1	1	-1.12540	16	13	13	12	4.73671	22	20	8	8	6.95100
8	1	1	20.86223	5	5	2	1	2.36758	16	13	13	13	-57.36852	22	20	9	9	0.85216
8	2	1	2.79931	5	5	2	2	-2.03268	16	14	1	1	-85.95324	22	20	10	10	6.65213
8	2	2	-7.56158	5	5	3	1	-6.77409	16	14	2	2	57.30213	22	20	11	11	6.87403
8	3	1	1.48205	5	5	3	2	4.56462	16	14	3	3	-2.81721	22	20	12	12	3.25535
8	3	2	-8.23443	5	5	3	3	-15.65668	16	14	4	4	-0.37236	22	20	13	13	-6.99015
8	3	3	10.73316	5	5	4	1	1.05473	16	14	5	5	3.20151	22	20	14	14	0.21796
8	4	1	-4.41616	5	5	4	3	3.68783	16	14	6	6	1.20673	22	20	15	15	1.19779
8	4	2	12.53757	5	5	4	4	-2.11016	16	14	7	7	0.84893	22	20	16	16	-4.07851
8	4	3	-34.85019	5	5	5	1	-1.22858	16	14	10	10	-3.29687	22	20	17	17	-19.13778
8	4	4	13.30519	5	5	5	2	1.54510	16	14	12	12	12.16848	22	20	18	18	2.68834
8	5	1	8.93089	5	5	5	3	-1.39947	16	14	13	13	-33.82586	22	20	19	19	-6.79994
8	5	2	-14.97205	5	5	5	4	-2.33157	16	14	14	12	-27.47463	22	20	20	17	1.53635
8	5	3	46.36683	5	5	5	5	8.46589	16	14	14	13	-24.38424	22	20	20	18	-11.25207
8	5	4	-56.05355	6	1	1	1	-5.12140	16	14	14	14	52.39743	22	20	20	19	9.64882
8	5	5	3.13591	6	2	1	1	0.50281	16	15	1	1	-47.55537	22	20	20	20	-5.62276
8	6	1	-1.63870	6	2	2	1	-4.27699	16	15	2	2	-77.09098	22	21	1	1	5.59061
8	6	2	5.67529	6	2	2	2	31.44795	16	15	3	3	36.94379	22	21	2	2	-79.84456
8	6	3	-20.27332	6	3	1	1	-1.67470	16	15	4	4	-1.43918	22	21	3	3	27.44542
8	6	4	26.45198	6	3	2	2	9.66493	16	15	5	5	-3.87399	22	21	4	4	-2.67888
8	6	5	-8.60423	6	3	3	1	-8.22901	16	15	6	6	-0.67671	22	21	5	5	-1.56660
8	6	6	-2.25308	6	3	3	2	8.72301	16	15	8	8	-3.88252	22	21	6	6	-0.17025
8	7	1	-6.27147	6	3	3	3	-14.17200	16	15	9	9	-0.58659	22	21	7	7	-0.23684
8	7	2	-2.75848	6	4	1	1	0.37984	16	15	10	10	-50.69672	22	21	8	8	-12.61735
8	7	4	-17.43209	6	4	2	2	-0.68183	16	15	11	11	-17.82620	22	21	9	9	-3.68220
8	7	5	27.69592	6	4	3	3	-4.60578	16	15	12	12	-8.42401	22	21	10	10	-8.40965
8	7	6	-2.54994	6	4	4	1	1.62413	16	15	13	13	36.84183	22	21	12	12	-2.46912
8	7	7	5.47454	6	4	4	2	0.91566	16	15	14	14	52.16516	22	21	13	13	9.81294
8	8	1	55.89882	6	4	4	3	2.14734	16	15	15	12	-36.62213	22	21	14	14	1.92783
8	8	2	-32.76312	6	4	4	4	-11.66169	16	15	15	13	-46.54161	22	21	15	15	-2.32147
8	8	3	110.21877	6	5	1	1	-0.09626	16	15	15	14	9.30514	22	21	17	17	48.99794
8	8	4	17.08924	6	5	2	2	1.04659	16	15	15	15	-4.49017	22	21	18	18	1.35333
8	8	5	-20.24921	6	5	3	3	5.60032	16	16	1	1	-44.53831	22	21	19	19	1.59530
8	8	6	25.61859	6	5	4	4	-2.52402	16	16	2	1	3.62479	22	21	20	20	-0.74293
8	8	7	-10.33259	6	5	5	1	1.58761	16	16	2	2	-78.76971	22	21	21	17	0.29145
8	8	8	33.67824	6	5	5	2	1.77004	16	16	3	1	2.36602	22	21	21	18	6.83657
9	1	1	-10.85710	6	5	5	3	1.32551	16	16	3	2	-13.92142	22	21	21	19	-8.07924
9	2	1	-0.94020	6	5	5	4	2.76931	16	16	3	3	-45.24354	22	21	21	20	-1.25361
9	2	2	-19.87901	6	5	5	5	-4.73380	16	16	4	2	-0.55062	22	21	21	21	5.63867
9	3	1	9.09272	6	6	1	1	-0.40152	16	16	4	3	-3.45690	22	22	1	1	-7.74037
9	3	2	-8.18682	6	6	2	1	0.16404	16	16	4	4	-11.03103	22	22	2	1	12.93933
9	3	3	2.19049	6	6	2	2	0.12980	16	16	5	1	0.67195	22	22	2	2	-79.99778
9	4	1	18.78866	6	6	3	1	-0.78995	16	16	5	2	-3.75921	22	22	3	1	-12.41819
9	4	2	-12.21512	6	6	3	2	0.64462	16	16	5	3	0.23975	22	22	3	2	-16.53623
9	4	3	18.72027	6	6	3	3	-1.85237	16	16	5	4	1.10283	22	22	3	3	-46.11543
9	4	4	-4.36460	6	6	4	1	1.01022	16	16	5	5	-15.71572	22	22	4	1	0.90627
9	5	1	-16.56811	6	6	4	2	0.98262	16	16	6	2	-5.23925	22	22	4	2	-0.53859
9	5	2	-4.95062	6	6	4	3	1.82127	16	16	6	4	-4.11756	22	22	4	3	1.90543
9	5	3	-26.46714	6	6	4	4	-1.79573	16	16	6	5	-2.18504	22	22	4	4	5.71989
9	5	4	16.70331	6	6	5	1	-0.40787	16	16	6	6	-7.12155	22	22	5	1	-0.25653
9	5	5	41.88242	6	6	5	2	1.45869	16	16	7	1	-1.32330	22	22	5	2	-0.97816
9	6	1	1.02653	6	6	5	3	1.03473	16	16	7	4	7.48164	22	22	5	3	-1.40844
9	6	2	-7.25362	6	6	5	4	-4.10979	16	16	7	5	1.70884	22	22	5	5	5.09244
9	6	3	4.74012	6	6	5	5	-1.86143	16	16	7	6	1.63545	22	22	6	1	0.66180
9	6	4	3.20005	6	6	6	1	-0.49838	16	16	7	7	-9.02044	22	22	6	2	-2.47202
9	6	5	8.06098	6	6	6	2	1.30151	16	16	8	1	-0.49565	22	22	6	3	0.47518
9	7	1	-4.84202	6	6	6	3	-0.33954	16	16	8	3	2.46803	22	22	6	4	0.49827
9	7	2	1.27571	6	6	6	4	-0.52797	16	16	8	4	-3.00989	22	22	6	5	0.51658
9	7	3	3.52894	6	6	6	5	-1.03336	16	16	8	5	6.71511	22	22	6	6	2.69594
9	7	4	-28.05564	6	6													

I	J	K	F(I,J,K)	I	J	K	L	F(I,J,,K,L)	I	J	K	L	F(I,J,K,L)	I	J	K	L	F(I,J,K,L)
23	20	5	-7.66216	14	13	13	13	40.90493	21	20	2	2	25.79805	24	24	9	8	-2.50748
23	20	6	13.27859	14	14	1	1	-205.57681	21	20	3	3	17.97396	24	24	9	9	1.62249
23	20	7	-9.63117	14	14	2	1	-44.02813	21	20	4	4	3.28040	24	24	10	10	1.90339
23	20	8	19.92695	14	14	2	2	-64.14696	21	20	5	5	-2.60067	24	24	11	10	-0.68822
23	20	9	2.30839	14	14	3	1	78.18921	21	20	6	6	0.11545	24	24	11	11	4.60862
23	21	1	-49.76850	14	14	3	2	-0.41667	21	20	7	7	2.42967	24	24	12	12	1.51851
23	21	2	-62.07622	14	14	3	3	-34.98647	21	20	8	8	-7.39249	24	24	13	12	0.56503
23	21	3	27.50636	14	14	4	1	11.46317	21	20	9	9	-0.91267	24	24	13	13	1.19780
23	21	4	-2.04369	14	14	4	2	2.07747	21	20	10	10	-5.36123	24	24	14	12	-3.40853
23	21	5	13.71436	14	14	4	3	-4.00451	21	20	11	11	-1.49660	24	24	14	14	7.63766
23	21	6	8.58864	14	14	4	4	-8.60970	21	20	12	12	-0.79990	24	24	15	13	-1.67519
23	21	7	5.88838	14	14	5	1	-12.13027	21	20	13	13	-5.01216	24	24	15	14	5.32348
23	21	9	5.13109	14	14	5	2	-5.35149	21	20	14	14	0.66206	24	24	15	15	6.59334
23	22	1	-5.91041	14	14	5	3	4.20304	21	20	15	15	-4.05401	24	24	16	12	-2.38774
23	22	2	-32.78326	14	14	5	4	-0.87672	21	20	16	16	-1.63811	24	24	16	13	-1.13364
23	22	3	-32.66506	14	14	5	5	-2.98256	21	20	17	17	20.27294	24	24	16	14	0.73231
23	22	4	-11.67116	14	14	6	1	3.17535	21	20	18	18	1.17814	24	24	16	16	-1.33562
23	22	5	10.71833	14	14	6	2	-1.96018	21	20	19	19	1.75549	24	24	17	17	-12.91387
23	22	6	4.58137	14	14	6	3	-2.80008	21	20	20	17	-1.83749	24	24	18	17	1.32812
23	22	7	-3.12229	14	14	6	4	1.71815	21	20	20	18	-1.98914	24	24	18	18	-1.01272
23	22	8	-10.57456	14	14	6	5	-0.81276	21	20	20	19	-0.67893	24	24	19	17	0.25645
23	22	9	-5.07049	14	14	6	6	-2.68676	21	20	20	20	8.17674	24	24	19	18	3.88247
23	23	1	203.01063	14	14	7	1	-8.67246	21	21	1	1	-28.72164	24	24	19	19	-3.09557
23	23	2	26.47876	14	14	7	2	-1.94657	21	21	2	1	10.32806	24	24	20	17	0.80194
23	23	3	-69.56444	14	14	7	3	3.25585	21	21	2	2	-95.45087	24	24	20	18	2.15742
23	23	4	9.28566	14	14	7	4	-1.02116	21	21	3	1	-6.38535	24	24	20	19	5.08445
23	23	5	-13.22657	14	14	7	5	-0.36002	21	21	3	2	-18.19916	24	24	20	20	-9.04457
23	23	6	-3.33568	14	14	7	7	-2.31027	21	21	3	3	-54.58635	24	24	21	17	0.12737
23	23	7	-21.61564	14	14	8	1	2.20913	21	21	4	1	1.12783	24	24	21	18	1.27865
23	23	8	17.89508	14	14	8	2	0.72169	21	21	4	2	0.18095	24	24	21	19	1.89607
23	23	9	-27.44015	14	14	8	4	-0.48246	21	21	4	3	1.73835	24	24	21	20	-1.52393
24	12	10	5.64710	14	14	8	6	0.77393	21	21	4	4	0.71488	24	24	21	21	7.18235
24	12	11	1.39269	14	14	9	1	-2.54471	21	21	5	1	-0.90377	24	24	22	17	-0.20925
24	13	10	-3.46504	14	14	9	2	0.73109	21	21	5	2	-0.40838	24	24	22	18	2.58683
24	13	11	-2.33199	14	14	9	3	1.23111	21	21	5	3	-0.36251	24	24	22	19	-4.28213
24	14	10	-3.28256	14	14	9	4	-0.67746	21	21	5	4	-2.11817	24	24	22	20	2.05138
24	14	11	0.98244	14	14	9	5	-0.52002	21	21	5	5	2.58105	24	24	22	21	0.31549
24	15	10	-5.31380	14	14	9	6	0.32291	21	21	6	1	1.16496	24	24	22	22	4.56147
24	15	11	8.21603	14	14	9	7	-0.55755	21	21	6	2	-2.61858	24	24	23	18	-3.95528
24	16	11	8.73294	14	14	9	9	-2.26009	21	21	6	3	0.26983	24	24	23	19	-8.13196
24	17	1	1.62214	14	14	10	10	2.62010	21	21	6	4	1.05330	24	24	23	20	-3.49256
24	17	2	-4.99979	14	14	11	10	1.90677	21	21	6	5	-0.13767	24	24	23	21	-3.05490
24	17	3	13.84703	14	14	11	11	3.22644	21	21	6	6	1.65151	24	24	23	22	-1.42318
24	17	4	-22.22595	14	14	12	12	35.45306	21	21	7	1	-0.49149	24	24	23	23	20.28081
24	17	5	35.44745	14	14	13	12	6.14355	21	21	7	2	0.18031	24	24	24	17	0.54470
24	17	6	-16.29739	14	14	13	13	27.71495	21	21	7	3	-0.27340	24	24	24	18	-4.86022
24	17	7	2.43436	14	14	14	12	-68.56127	21	21	7	4	-0.11005	24	24	24	19	-0.88190
24	17	8	52.93155	14	14	14	13	-5.66820	21	21	7	5	0.31506	24	24	24	20	-2.89787
24	17	9	-26.90370	14	14	14	14	138.81685	21	21	7	6	-0.32363	24	24	24	21	-2.69677
24	18	1	-43.04636	15	12	1	1	54.24241	21	21	7	7	-0.51906	24	24	24	22	-2.84018
24	18	2	14.63074	15	12	2	2	-20.38769	21	21	8	1	-0.43443	24	24	24	23	9.86649
24	18	3	-3.60756	15	12	3	3	-58.66508	21	21	8	2	-0.37943	24	24	24	24	11.06285
24	18	4	6.91592	15	12	4	4	3.84914	21	21	8	3	0.39246					

Table S36: The quartic potential energy surface of Pyridazine. The calculation was done by using B3LYP/6-311++G(2d,2p) method. The force constants (F_I) are in cm⁻¹ units.

I J	F _I (I,J)	I J K	F _I (I,J,K)	I J K L	F _I (I,J,K,L)	I J K L	F _I (I,J,K,L)
1 1	3200.70313	24 18 5	-10.12243	14 14 4 2	-0.87024	21 21 9 1	1.55280
2 2	3175.14891	24 18 6	-17.61858	14 14 4 3	4.50664	21 21 9 2	4.63014
3 3	1608.51241	24 18 7	-63.53064	14 14 4 4	20.38354	21 21 9 3	0.51660
4 4	1481.58571	24 18 8	-11.92807	14 14 5 1	-4.00827	21 21 9 4	-4.67341
5 5	1177.34505	24 18 9	-5.00905	14 14 5 2	-0.56958	21 21 9 5	-3.38714
6 6	1173.32161	24 19 1	44.53643	14 14 5 3	-2.48236	21 21 9 6	-1.88026
7 7	1089.17819	24 19 2	44.84720	14 14 5 4	10.69347	21 21 9 7	-1.02769
8 8	1005.92048	24 19 4	5.75744	14 14 5 5	12.01382	21 21 9 8	0.20366
9 9	682.93268	24 19 5	0.96533	14 14 6 1	1.06851	21 21 9 9	-2.42931
10 10	1018.22908	24 19 6	-16.34774	14 14 6 2	4.42663	21 21 10 10	8.03445
11 11	942.76231	24 19 7	11.84004	14 14 6 3	7.23818	21 21 11 10	-14.70701
12 12	773.45213	24 19 8	-21.56119	14 14 6 4	-2.80399	21 21 11 11	24.13768
13 13	376.35638	24 19 9	20.37048	14 14 6 5	-8.41981	21 21 12 10	-0.16555
14 14	984.70497	24 20 1	-35.61233	14 14 6 6	4.88732	21 21 12 11	-2.43489
15 15	760.70948	24 20 2	59.81501	14 14 7 1	1.06822	21 21 12 12	-5.74944
16 16	374.68890	24 20 3	17.28551	14 14 7 2	-2.73530	21 21 13 10	2.76848
17 17	3187.76330	24 20 4	21.78742	14 14 7 3	4.58475	21 21 13 11	-5.54452
18 18	3170.54505	24 20 5	-32.21708	14 14 7 4	18.35774	21 21 13 12	4.15929
19 19	1602.52826	24 20 6	-10.64315	14 14 7 5	5.30815	21 21 13 13	-3.63882
20 20	1446.62251	24 20 7	-4.05701	14 14 7 6	2.55138	21 21 14 14	18.76783
21 21	1314.98529	24 20 8	-5.52067	14 14 7 7	11.25408	21 21 15 14	17.23309
22 22	1086.59894	24 20 9	6.86720	14 14 8 1	0.23693	21 21 15 15	14.18390
23 23	1062.87007	24 21 1	-26.15342	14 14 8 2	-1.44833	21 21 16 14	10.95788
24 24	637.32132	24 21 2	-79.91099	14 14 8 3	1.98197	21 21 16 15	6.79122
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I J K	F _I (I,J,K)	24 21 4	17.78116	14 14 8 5	0.71807	21 21 17 17	-42.50183
		24 21 5	-7.77016	14 14 8 6	0.45415	21 21 18 17	-64.20372
1 1 1	-1232.42693	24 21 6	-2.11239	14 14 8 7	3.70736	21 21 18 18	-97.86866
2 1 1	261.65798	24 21 7	0.42696	14 14 9 1	0.57147	21 21 19 17	0.20802
2 2 1	-500.53744	24 21 8	-15.78713	14 14 9 2	1.27939	21 21 19 18	0.31948
2 2 2	-1165.97845	24 21 9	8.56009	14 14 9 3	3.30079	21 21 19 19	20.50254
3 1 1	-21.60942	24 22 1	47.48185	14 14 9 4	-2.90244	21 21 20 17	0.53500
3 2 1	6.96956	24 22 2	16.30761	14 14 9 5	-5.83800	21 21 20 18	0.06147
3 2 2	-6.40272	24 22 3	0.94314	14 14 9 6	4.54820	21 21 20 19	17.03536
3 3 1	104.72881	24 22 4	13.08686	14 14 9 7	-0.95526	21 21 20 20	13.47523
3 3 2	-33.19945	24 22 5	13.74759	14 14 9 8	0.40168	21 21 21 17	5.83085
3 3 3	-193.22688	24 22 6	-18.56563	14 14 9 9	2.04839	21 21 21 18	8.89113
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4 2 1	0.83187	24 22 8	-4.21686	14 14 11 10	-51.89176	21 21 21 20	-9.24472
4 2 2	-22.38567	24 22 9	-5.57215	14 14 11 11	185.87595	21 21 21 21	40.57958
4 3 1	3.84269	24 23 1	-9.81709	14 14 12 10	7.47857	22 17 1 1	2.80588
4 3 2	37.18122	24 23 2	0.61020	14 14 12 11	-18.71835	22 17 2 2	1.99063
4 3 3	17.55009	24 23 3	-8.25588	14 14 12 12	12.36935	22 17 3 3	1.51587
4 4 1	54.90048	24 23 4	-17.30433	14 14 13 10	42.89780	22 17 4 4	1.39329
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4 4 3	25.76615	24 23 6	23.72194	14 14 13 12	7.61103	22 17 6 6	-2.20886
4 4 4	-34.25450	24 23 7	8.58606	14 14 13 13	19.08333	22 17 7 7	1.01637
5 1 1	-1.17253	24 23 8	0.42216	14 14 14 14	168.82627	22 17 8 8	-1.40144
5 2 1	2.05693	24 23 9	-9.21967	15 14 1 1	157.35004	22 17 9 9	-0.77770
5 2 2	-2.08161	24 24 1	22.28577	15 14 2 2	-157.72595	22 17 10 10	0.65976
5 3 1	-82.71564	24 24 2	30.47828	15 14 3 3	-7.86973	22 17 11 11	-1.77016
5 3 2	46.08322	24 24 3	14.26224	15 14 4 4	19.11338	22 17 12 12	0.50656
5 3 3	-65.37795	24 24 4	-10.01507	15 14 5 5	-10.50649	22 17 13 13	1.44175
5 4 1	20.20013	24 24 5	6.79684	15 14 6 6	-14.53355	22 17 14 14	3.48053
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5 5 3	-4.66523			15 14 12 12	0.90708	22 18 4 4	3.25916
5 5 4	-26.94357	1 1 1 1	454.99419	15 14 13 13	-16.82976	22 18 5 5	0.82035
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6 1 1	0.66240	2 2 1 1	91.28296	15 15 1 1	-330.01840	22 18 7 7	0.99265
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6 3 1	97.06318	3 1 1 1	9.89797	15 15 3 1	-3.58487	22 18 10 10	1.92301
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6 4 2	-21.95949	3 3 1 1	-55.33572	15 15 4 2	1.64372	22 18 14 14	2.80762
6 4 3	-60.80043	3 3 2 1	14.73219	15 15 4 3	3.30377	22 18 15 15	0.31902
6 4 4	39.63640	3 3 2 2	-14.07941	15 15 4 4	12.81345	22 18 16 16	-0.53508
6 5 1	-118.55848	3 3 3 1	-7.26334	15 15 5 1	-1.69153	22 18 17 17	-0.05205
6 5 2	37.17546	3 3 3 2	-0.57984	15 15 5 2	2.57923	22 18 18 17	1.98102
6 5 3	50.65341	3 3 3 3	48.44358	15 15 5 3	-18.76556	22 18 18 18	0.57532
6 5 4	-25.32504	4 1 1 1	10.16029	15 15 5 4	8.65987	22 19 1 1	-45.49825
6 5 5	-21.67644	4 2 1 1	-1.46157	15 15 5 5	35.95353	22 19 2 2	-29.29182
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6 6 2	-27.57516	4 2 2 2	8.00252	15 15 6 2	4.80505	22 19 4 4	-0.81926
6 6 3	84.75960	4 3 1 1	-6.40232	15 15 6 3	18.71391	22 19 5 5	11.74517
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6 6 6	-192.92358	4 3 3 2	-1.03041	15 15 7 1	7.12467	22 19 8 8	-6.36886
7 1 1	30.20722	4 3 3 3	-0.41252	15 15 7 2	-1.37006	22 19 9 9	3.01446
7 2 1	-8.86130	4 4 1 1	-14.19080	15 15 7 3	9.78671	22 19 10 10	9.63971

I	J	K	F(I,J,K)	I	J	K	L	F(I,J,K,L)	I	J	K	L	F(I,J,K,L)	I	J	K	L	F(I,J,K,L)
9	7	7	-26.87796	7	3	3	1	4.45117	16	16	7	7	-1.28891	22	22	8	3	1.23585
9	8	1	12.73723	7	3	3	2	-3.69068	16	16	8	1	-0.40515	22	22	8	4	3.45960
9	8	2	-10.93800	7	3	3	3	-32.48486	16	16	8	2	-1.05656	22	22	8	5	-7.61669
9	8	3	-15.56334	7	4	1	1	-10.65011	16	16	8	3	7.49046	22	22	8	6	0.41025
9	8	4	22.59486	7	4	2	2	-90.89350	16	16	8	4	-3.97491	22	22	8	7	-2.67662
9	8	5	-22.56722	7	4	3	3	0.75705	16	16	8	5	2.45340	22	22	8	8	4.86916
9	8	6	1.95505	7	4	4	1	-0.33313	16	16	8	6	-0.43201	22	22	9	1	-1.76786
9	8	7	-13.38260	7	4	4	2	-1.33017	16	16	8	7	2.85517	22	22	9	2	1.94573
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9	9	2	-8.76266	7	4	4	4	20.03131	16	16	9	2	-1.09224	22	22	9	4	-4.01677
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9	9	5	-2.45520	7	5	3	3	-17.48177	16	16	9	5	-4.18827	22	22	9	7	4.30649
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12	11	8	-1.99807	8	2	1	1	-1.56033	17	17	8	1	7.11136	23	17	8	8	0.43904
12	11	9	-6.52508	8	2	2	1	4.27166	17	17	8	2	1.59549	23	17	9	9	-0.83527
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12	12	6	15.62785	8	3	3	3	8.36246	17	17	8	8	-3.46786	23	17	16	16	-0.65491
12	12	7	-7.72752	8	4	1	1	-2.52394	17	17	9	1	-0.57539	23	17	17	17	0.55639
12	12	8	10.97864	8	4	2	2	-18.23601	17	17	9	2	0.29199	23	18	1	1	0.93248
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13	11	2	-110.85728	8	5	5	3	0.91633	17	17	12	10	-24.14952	23	18	12	12	-0.61073
13	11	3	-8.37739	8	5													

I J K	FI(I,J,K)	I J K L	FI(I,J,K,L)	I J K L	FI(I,J,K,L)	I J K L	FI(I,J,K,L)
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13 12 5	-13.40071	8 6 6 4	-7.30305	17 17 16 15	35.06168	23 19 4 4	6.48727
13 12 6	-20.96511	8 6 6 5	-3.87803	17 17 16 16	-39.27599	23 19 5 5	-3.96099
13 12 7	-30.78879	8 6 6 6	-4.62163	17 17 17 17	318.33312	23 19 6 6	-9.46994
13 12 8	-6.06927	8 7 1 1	-8.06216	18 17 1 1	-206.98396	23 19 7 7	-1.83493
13 12 9	4.41488	8 7 2 2	-12.69653	18 17 2 2	207.41058	23 19 8 8	6.02122
13 13 1	79.24014	8 7 3 3	-1.39590	18 17 3 3	24.20489	23 19 9 9	-2.40058
13 13 2	-13.09084	8 7 4 4	9.87547	18 17 4 4	-68.01955	23 19 10 10	-4.25701
13 13 3	67.81091	8 7 5 5	0.27833	18 17 5 5	38.32711	23 19 11 11	-0.74912
13 13 4	-39.86347	8 7 6 6	11.40332	18 17 6 6	36.17971	23 19 13 13	-1.72109
13 13 5	38.22473	8 7 7 1	-0.67085	18 17 7 7	-23.18793	23 19 14 14	-0.85236
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13 13 7	-44.04475	8 7 7 3	7.90777	18 17 9 9	11.51051	23 19 16 16	0.93094
13 13 8	64.95443	8 7 7 4	-7.01319	18 17 10 10	68.48556	23 19 17 17	12.87815
13 13 9	-5.05277	8 7 7 5	1.51285	18 17 11 11	-75.09675	23 19 18 18	5.85263
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14 14 7	4.97482	8 8 3 1	0.48332	18 17 17 17	-100.77151	23 20 3 3	5.04197
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20	18	4	-75.78603	10	10	6	5	-14.49329	19	19	16	14	13.98735	24	17	5	5	2.57269
20	18	5	-114.90160	10	10	6	6	13.50379	19	19	16	15	3.17975	24	17	6	6	1.23681
20	18	6	80.77590	10	10	7	1	-0.18133	19	19	16	16	-23.25691	24	17	7	7	1.66222
20	18	7	-21.90680	10	10	7	2	-1.26904	19	19	17	17	-35.08162	24	17	8	8	-0.22290
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20	18	9	54.97199	10	10	7	4	7.89635	19	19	18	18	-46.10340	24	17	11	11	-0.15641
20	19	1	-57.21761	10	10	7	5	-2.69460	19	19	19	17	3.10999	24	17	12	12	-0.48792
20	19	2	75.89891	10	10	7	6	4.37499	19	19	19	18	5.16867	24	17	13	13	-0.40739
20	19	3	16.59500	10	10	7	7	3.86105	19	19	19	19	27.15488	24	17	14	14	1.09021
20	19	4	43.12804	10	10	8	1	-0.86136	20	17	1	1	3.72555	24	17	15	15	0.57387
20	19	5	-30.95463	10	10	8	3	1.09921	20	17	2	2	1.53897	24	17	16	16	0.59095
20	19	6	-117.26260	10	10	8	4	1.75011	20	17	3	3	1.96113	24	17	17	17	-1.13473
20	19	7	-5.18446	10	10	8	5	-2.11446	20	17	4	4	0.34200	24	18	1	1	-0.46735
20	19	8	-1.36679	10	10	8	6	2.33293	20	17	5	5	-0.99379	24	18	2	2	-1.02340
20	19	9	-17.40555	10	10	8	7	3.10868	20	17	6	6	0.21588	24	18	3	3	-0.95096
20	20	1	160.99761	10	10	8	8	-0.35480	20	17	7	7	1.53245	24	18	4	4	-0.19098
20	20	2	-9.96915	10	10	9	1	-0.94831	20	17	9	9	1.20177	24	18	5	5	-2.36863
20	20	3	28.55144	10	10	9	2	1.12207	20	17	10	10	-0.92982	24	18	6	6	-0.87851
20	20	4	14.62230	10	10	9	3	7.43069	20	17	11	11	0.52408	24	18	7	7	-1.00451
20	20	5	-17.10596	10	10	9	4	-0.68641	20	17	12	12	0.21176	24	18	8	8	-0.31650
20	20	6	-60.08877	10	10	9	5	-9.74757	20	17	13	13	-2.19633	24	18	9	9	0.35493
20	20	7	47.91693	10	10	9	6	9.26219	20	17	14	14	-1.83577	24	18	10	10	-0.93215
20	20	8	-37.57282	10	10	9	7	2.29880	20	17	15	15	-3.98396	24	18	11	11	-0.79926
20	20	9	17.42220	10	10	9	8	1.37648	20	17	16	16	1.60978	24	18	12	12	0.21767
21	14	10	-8.31321	10	10	9	9	3.87226	20	17	17	17	5.62888	24	18	13	13	0.51785
21	14	11	-3.22579	10	10	10	10	377.69198	20	18	1	1	-1.22979	24	18	14	14	-0.67318
21	14	12	-2.06443	11	10	1	1	-134.20909	20	18	2	2	3.42982	24	18	15	15	-1.54821
21	14	13	10.74976	11	10	2	2	133.77419	20	18	3	3	1.42306	24	18	16	16	0.25178
21	15	10	8.39458	11	10	3	3	6.72904	20	18	4	4	1.77276	24	18	17	17	-0.25867
21	15	11	-6.98055	11	10	4	4	-15.17443	20	18	5	5	0.74563	24	18	18	17	-0.61623
21	15	12	-2.76111	11	10	5	5	7.82087	20	18	6	6	-1.37418	24	18	18	18	-0.88981
21	15	13	17.86920	11	10	6	6	10.47064	20	18	7	7	0.84360	24	19	1	1	-15.29320
21	16	10	-3.42137	11	10	7	7	-6.77606	20	18	9	9	-0.31807	24	19	2	2	-31.27792
21	16	11	1.13883	11	10	9	9	3.77605	20	18	10	10	1.71453	24	19	3	3	6.64545
21	16	12	-26.28990	11	10	10	10	62.77350	20	18	11	11	-0.61969	24	19	4	4	15.82385
21	16	13	32.63371	11	11	1	1	-125.20179	20	18	12	12	0.24876	24	19	5	5	10.21316
21	17	1	-8.22288	11	11	2	1	-46.95122	20	18	13	13	0.72780	24	19	6	6	10.01778
21	17	2	-1.44431	11	11	2	2	-259.48145	20	18	14	14	2.34464	24	19	7	7	9.06615
21	17	3	18.65120	11	11	3	1	-0.77814	20	18	15	15	1.68714	24	19	8	8	3.58007
21	17	4	86.63314	11	11	3	2	-3.40972	20	18	16	16	-1.29290	24	19	9	9	2.22774
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21	17	6	-8.08977	11	11	4	1	-3.28941	20	18	18	17	2.52209	24	19	11	11	10.23338
21	17	7	66.55590	11	11	4	2	-0.75366	20	18	18	18	2.14073	24	19	12	12	-2.15990
21	17	8	13.62793	11	11	4	3	4.99434	20	19	1	1	49.37341	24	19	13	13	-1.21923
21	17	9	-17.00172	11	11	4	4	23.83290	20	19	2	2	-34.60137	24	19	14	14	8.49069
21	18	1	3.61099	11	11	5	1	3.92981	20	19	3	3	0.88807	24	19	15	15	11.78209
21	18	2	-8.96163	11	11	5	2	0.10507	20	19	4	4	4.72619	24	19	16	16	1.37751
21	18	3	29.87648	11	11	5	3	-3.41032	20	19	5	5	-8.76498	24	19	17	17	-19.80394
21	18	4	131.18594	11	11	5	4	13.79911	20	19	6	6	7.67165	24	19	18	18	-27.47135
21	18	5	68.28238	11	11	5	5	14.36126	20	19	7	7	3.10221	24	19	19	17	1.78864
21	18	6	-8.22182	11	11	6	1	2.01266	20	19	8	8	-2.52676	24	19	19	18	0.66226
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21	18	8	22.43567	11	11	6	3	6.78733	20	19	10	10	5.08091	24	20	1	1	27.70047
21	18	9	-19.29008	11	11	6	4	-2.92417	20	19	11	11	3.46077	24	20	2	2	-21.92881
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21	19	2	-91.45970	11	11	6	6	2.30079	20	19	13	13	-1.77895	24	20	4	4	11.09363
21	19	3	43.66265	11	11	7	1	-1.25893	20	19	14	14	2.08708	24	20	5	5	-5.67318
21	19	4	9.65303	11	11	7	2	-1.13704	20	19	15	15	-9.28934	24	20	6	6	-3.99763
21	19	5	-26.45362	11	11	7	3	4.58568	20	19	16	16	-3.28999	24	20	7	7	2.14128
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21	19	9	9.40408	11	11	7	7	13.55186	20	19	19	18	1.09248	24	20	11	11	3.52688
21	20	1	-21.88330	11	11	8	1	-3.06537	20	19	19	19	-1.69177	24	20	12	12	-0.59390
21	20	2	-77.54100	11	11	8	2	-3.23197	20	20	1	1	-127.21983	24	20	13	13	-1.69984
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21	20	5	-36.36851	11	11	8	5	0.95258	20	20	3	1	1.74796	24	20	16	16	1.02688
21	20	6	-88.34368	11	11	8	6	1.80692	20	20	3	2	-2.84654	24	20	17	17	15.46181
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21	20	8	-15.60879	11	11	8	8	-0.92970	20	20	4	1	-1.68667	24	20	19	19	4.54687
21	20	9	15.12325	11	11	9	1	-0.59160	20	20	4	2	-1.14045	24	20	20	17	3.10574
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21	21	2	146.45602	11	11	9	3	2.81816	20	20	4	4	8.17965	24	20	20	19	8.16531
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22	16	13	-15.41991	12	11	1	1	-9.99926	20	20	8	2	0.59493	24	21	18	18	38.98626
22	17	1	-11.80363	12	11	2	2	39.02930	20	20	8	3	2.47256	24	21	19	19	-3.12661
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22	17	5	-132.58350	12	11	6	6	-3.76795	20	20	8	8	0.83865	24	21	21	19	11.39301
22	17	6	89.90153	12	11	7	7	0.75651	20	20	9	1	-0.68214	24	21	21	20	7.64876
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22	17	9	60.87027	12	11	10	10	2.91150	20	20	9	4	-3.70412	24	22	2	2	-18.18627
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22	19	6	-102.43640	12	12	5	4	3.79333	20	20	13	13	-4.75673	24	22	18	18	-20.40615
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22	20	9	8.77622	12	12	7	6	6.26578	20	20	19	18	2.11741	24	23	2	2	-0.19666
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22	21	2	-54.00618	12	12	8	1	0.46197	20	20	20	17	-0.05513	24	23	4	4	-0.62623
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22	21	5	-52.80811	12	12	8	5	-0.36174	20	20	20	20	34.50834	24	23	7	7	0.89078
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22	21	7	-16.63466	12	12	8	7	-3.54002	21	17	2	2	4.13991	24	23	9	9	-0.83011
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22	21	9	18.40211	12	12	9	2	-0.40520	21	17	4	4	1.63350	24	23	11	11	-0.20825
22	22	1	122.90416	12	12	9	3	-1.90068	21	17	5	5	0.52743	24	23	12	12	-0.22431
22	22	2	-21.66351	12	12	9	4	1.01736	21	17	6	6	-0.66521	24	23	14	14	-0.95330
22	22	3	30.37648	12	12	9	5	-0.50079	21	17	7	7	-0.66615	24	23	15	15	-1.02887
22	22	4	-25.90034	12	12	9	6	1.27770	21	17	9	9	-0.43049	24	23	16	16	-1.18793
22	22	5	39.12066	12	12	9	7	-0.71025	21	17	10	10	-2.47185	24	23	17	17	7.43954
22	22	6	27.83254	12	12	9	8	-0.29129	21	17	11	11	0.28004	24	23	18	18	2.36394
22	22	7	43.02728	12	12	9	9	-1.93782	21	17	12	12	-0.12252	24	23	19	19	0.69830
22	22	8	-54.16961	12	12	10	10	73.76670	21	17	13	13	0.88045	24	23	20	20	-4.03836
22	22	9	26.52070	12	12	11	10	-7.95727	21	17	14	14	-1.51914	24	23	21	21	-0.68993
23	14	10	-6.57533	12	12	11	11	15.36455	21	17	15	15	-1.23795	24	23	22	22	-2.67896
23	14	11	-20.67910	12	12	12	10	-55.61802	21	17	16	16	-0.96758	24	23	23	17	0.49531
23	14	12	-8.32470	12	12	12	11	8.77457	21	17	17	17	3.72298	24	23	23	18	-0.30368
23	14	13	12.75161	12	12	12	12	52.22124	21	18	1	1	-0.46095	24	23	23	19	2.49245
23	15	10	19.24057	13	10	1	1	-102.43358	21	18	2	2	4.54372	24	23	23	22	0.18961
23	15	11	-0.67345	13	10	2	2	-35.13407	21	18	3	3	-1.27141	24	23	23	23	-4.11569
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23	16	11	23.54431	13	10	6	6	8.00415	21	18	7	7	-0.11156	24	24	3	1	1.45611
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23	16	13	1.34810	13	10	8	8	4.39811	21	18	10	10	0.88359	24	24	3	3	-9.68540
23	17	1	-2.57718	13	10	9	9	2.83979	21	18	11	11	1.41336	24	24	4	1	0.34071
23	17	2	-0.69878	13	10	10	10	26.48905	21	18	13	13	1.74937	24	24	4	3	4.12377
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23	17	4	-6.83282	13	11	2	2	35.98379	21	18	16	16	-1.34125	24	24	5	1	-0.53524
23	17	5	44.45331	13	11	3	3	9.80672	21	18	17	17	1.01717	24	24	5	2	0.49107
23	17	6	-34.70010	13	11	4	4	-6.48363	21	18	18	17	3.64592	24	24	5	3	-3.08366
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I	J	K	F(I,J,K)	I	J	K	L	F(I,J,K,L)	I	J	K	L	F(I,J,K,L)	I	J	K	L	F(I,J,K,L)
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23	19	3	17.24840	13	12	7	7	-2.56691	21	19	14	14	-13.80896	24	24	7	7	-0.91457
23	19	4	-19.22076	13	12	8	8	6.34866	21	19	15	15	-9.62010	24	24	8	3	-1.24830
23	19	5	34.64650	13	12	9	9	-1.89296	21	19	16	16	-14.77015	24	24	8	4	3.77801
23	19	6	63.63074	13	12	10	10	33.55299	21	19	17	17	26.63527	24	24	8	6	3.12537
23	19	7	-7.49785	13	12	11	11	8.68907	21	19	18	18	59.34022	24	24	8	7	-1.63061
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23	20	2	-15.12398	13	13	1	1	-45.15448	21	20	1	1	3.25573	24	24	9	5	-2.38040
23	20	3	-43.19843	13	13	2	1	11.79947	21	20	2	2	63.39594	24	24	9	6	0.69808
23	20	4	12.48865	13	13	2	2	-11.69599	21	20	3	3	1.02921	24	24	9	7	1.08244
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23	20	6	25.50017	13	13	3	2	-1.05879	21	20	5	5	0.81528	24	24	10	10	2.72755
23	20	7	-19.15221	13	13	3	3	-30.64186	21	20	6	6	18.27402	24	24	11	10	-2.23161
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23	20	9	-3.52267	13	13	4	2	2.59935	21	20	8	8	-0.30290	24	24	12	10	1.64663
23	21	1	-1.43546	13	13	4	3	7.13534	21	20	9	9	-1.94830	24	24	12	11	-1.39105
23	21	2	-4.58169	13	13	4	4	-16.48169	21	20	10	10	-4.16530	24	24	12	12	-2.50469
23	21	3	-24.00153	13	13	5	1	-0.22090	21	20	11	11	-12.40156	24	24	13	10	2.73847
23	21	4	-5.31169	13	13	5	2	0.17761	21	20	12	12	-3.94334	24	24	13	11	-0.38783
23	21	5	15.88710	13	13	5	3	-12.06555	21	20	13	13	-0.65704	24	24	13	12	-1.50564
23	21	6	49.96721	13	13	5	4	6.85580	21	20	14	14	-12.27352	24	24	13	13	4.28129
23	21	7	-25.03980	13	13	5	5	-7.04499	21	20	15	15	-6.93840	24	24	14	14	3.17970
23	21	8	-3.43889	13	13	6	1	1.48624	21	20	16	16	-9.99132	24	24	15	14	2.75341
23	21	9	-3.76034	13	13	6	2	-0.90409	21	20	17	17	18.72186	24	24	15	15	5.09690
23	22	1	-47.71538	13	13	6	3	2.81761	21	20	18	18	47.99016	24	24	16	14	1.91744
23	22	2	9.41967	13	13	6	4	1.10959	21	20	20	17	-2.87271	24	24	16	15	-0.78966
23	22	3	-26.77303	13	13	6	5	-3.42471	21	20	20	18	-0.84704	24	24	16	16	-3.18684
23	22	4	26.19416	13	13	6	6	-15.49463	21	20	20	19	1.31941	24	24	17	17	-12.59816
23	22	5	-25.17381	13	13	7	1	-0.76846	21	20	20	20	0.69179	24	24	18	17	-6.92663
23	22	6	22.68976	13	13	7	2	1.08415	21	21	1	1	-12.87761	24	24	18	18	-18.74880
23	22	7	-6.90652	13	13	7	3	10.87368	21	21	2	1	-39.99806	24	24	19	17	1.10147
23	22	8	18.69889	13	13	7	4	4.27751	21	21	2	2	-127.45015	24	24	19	18	-0.28306
23	22	9	-17.22119	13	13	7	5	4.40277	21	21	3	1	-1.43409	24	24	19	19	0.62622
23	23	1	8.92899	13	13	7	6	10.61511	21	21	3	2	-3.35462	24	24	20	17	-1.09782
23	23	2	-7.04659	13	13	7	7	-23.05271	21	21	3	3	2.04780	24	24	20	18	0.79615
23	23	3	22.37847	13	13	8	1	-0.84763	21	21	4	1	2.31158	24	24	20	19	0.99242
23	23	4	-23.67367	13	13	8	2	0.56020	21	21	4	2	6.80837	24	24	20	20	2.67259
23	23	5	15.90795	13	13	8	3	-7.03352	21	21	4	3	9.22347	24	24	21	17	0.46944
23	23	6	-23.92133	13	13	8	4	7.04572	21	21	4	4	34.30807	24	24	21	18	0.46218
23	23	7	11.34896	13	13	8	5	-2.76552	21	21	5	1	1.79762	24	24	21	19	-5.22562
23	23	8	-27.36826	13	13	8	6	10.42821	21	21	5	2	3.96207	24	24	21	20	-4.22993
23	23	9	2.39134	13	13	8	7	-7.12701	21	21	5	3	-0.48504	24	24	21	21	8.32643
24	14	10	6.59077	13	13	8	8	-19.07696	21	21	5	4	16.13254	24	24	22	17	0.66573
24	14	11	0.75151	13	13	9	1	0.84422	21	21	5	5	15.84931	24	24	22	19	3.86936
24	14	12	-4.80143	13	13	9	4	0.67044	21	21	6	1	1.70464	24	24	22	20	-1.10739
24	14	13	9.58440	13	13	9	5	-3.05022	21	21	6	2	6.03588	24	24	22	21	-3.44739
24	15	10	-8.04366	13	13	9	6	0.64476	21	21	6	3	-6.06166	24	24	22	22	2.60329
24	15	12	5.03760	13	13	9	7	3.16601	21	21	6	4	-10.80115	24	24	23	17	0.29885
24	15	13	12.06818	13	13	9	8	0.83379	21	21	6	5	4.96504	24	24	23	18	0.52301
24	16	10	5.93627	13	13	9	9	-4.41178	21	21	6	6	15.47739	24	24	23	19	0.97480
24	16	12	-3.07426	13	13	10	10	48.29103	21	21	7	1	0.39944	24	24	23	20	0.73686
24	16	13	14.65720	13	13	11	10	17.50967	21	21	7	2	1.41402	24	24	23	21	-0.20521
24	17	1	1.61804	13	13	11	11	20.63575	21	21	7	3	3.99927	24	24	23	22	-2.58867
24	17	2	-1.66786	13	13	12	10	-5.56628	21	21	7	4	28.09905	24	24	23	23	-3.66313
24	17	3	11.61341	13	13	12	12	12.27810	21	21	7	5	12.01788	24	24	24	17	0.15488
24	17	4	-52.11603	13	13	13	10	8.23025	21	21	7	6	-3.43523	24	24	24	18	0.30133
24	17	5	-64.39668	13	13	13	11	5.06288	21	21	7	7	14.97792	24	24	24	19	3.43207
24	17	6	37.29770	13	13	13	13	55.13462	21	21	8	1	0.12612	24	24	24	20	1.61313
24	17	7	-12.99453	14	14	1	1	-117.61932	21	21	8	2	0.25909	24	24	24	21	-3.90364
24	17	8	0.75906	14	14	2	1	-37.25147	21	21	8	3	-1.86478	24	24	24	22	2.97914
24	17	9	26.44017	14	14	2	2	-227.28365	21	21	8	4	7.18024	24	24	24	23	-1.18696
24	18	1	-2.01952	14	14	3	1	-1.42170	21	21	8	5	5.21682	24	24	24	24	6.35496
24	18	2	-0.82217	14	14	3	2	-3.99839	21	21	8	6	7.97933					
24	18	3	-33.42973	14	14	3	3	1.08129	21	21	8	7	2.31413					
24	18	4	-75.10005	14	14	4	1	-0.70145	21	21	8	8	1.84527					

Table S37: The quartic potential energy surface of Pyridazine-d4 The calculation was done by using B3LYP/6-311++G(2d,2p) method. The force constants (F_I) are in cm⁻¹ units.

I J	F(I,J)	I J K	F(I,J,K)	I J K L	F(I,J,K,L)	I J K L	F(I,J,K,L)
1 1	2375.60974	24 17 9	36.86225	13 13 13 11	4.96428	21 21 7 2	-0.79320
2 2	2346.20079	24 18 1	8.67710	13 13 13 12	2.59283	21 21 7 3	-0.57720
3 3	1563.49343	24 18 2	-4.16742	13 13 13 13	46.52253	21 21 7 4	-3.28557
4 4	1346.45706	24 18 3	-13.86587	14 14 1 1	-54.08337	21 21 7 5	-0.43522
5 5	1149.84129	24 18 4	36.72155	14 14 2 1	-18.07776	21 21 7 6	1.00151
6 6	984.19758	24 18 5	3.02876	14 14 2 2	-95.90422	21 21 7 7	5.20971
7 7	872.00208	24 18 6	7.35759	14 14 3 1	-1.99193	21 21 8 1	0.20233
8 8	847.31932	24 18 7	-57.95572	14 14 3 2	3.64214	21 21 8 2	-0.38728
9 9	654.74241	24 18 8	43.83244	14 14 3 3	-3.67622	21 21 8 3	-1.03187
10 10	854.95643	24 18 9	-15.97230	14 14 4 1	1.75069	21 21 8 4	0.71099
11 11	748.79764	24 19 1	31.51510	14 14 4 2	0.86840	21 21 8 5	0.63827
12 12	692.43066	24 19 2	24.69839	14 14 4 3	-0.81884	21 21 8 6	0.47102
13 13	343.22178	24 19 3	-4.41193	14 14 4 4	-1.21011	21 21 8 7	-0.37261
14 14	807.38673	24 19 4	-23.03301	14 14 5 1	1.77323	21 21 8 8	1.20085
15 15	570.20958	24 19 5	20.34325	14 14 5 2	-1.57882	21 21 9 2	0.43481
16 16	328.98380	24 19 6	-18.27203	14 14 5 3	-2.33947	21 21 9 3	-0.74632
17 17	2358.69454	24 19 7	5.56391	14 14 5 4	1.12583	21 21 9 4	-0.24748
18 18	2339.89984	24 19 8	8.35460	14 14 5 5	-5.19709	21 21 9 5	0.56696
19 19	1559.71882	24 19 9	18.11512	14 14 6 1	-2.47769	21 21 9 6	0.55751
20 20	1302.65706	24 20 1	-29.65881	14 14 6 2	-2.73939	21 21 9 7	-0.20439
21 21	1053.72010	24 20 2	25.21231	14 14 6 3	1.96919	21 21 9 8	-1.12822
22 22	1002.86571	24 20 3	11.38172	14 14 6 4	1.13363	21 21 9 9	-1.02054
23 23	851.01632	24 20 4	-36.35149	14 14 6 5	0.27755	21 21 10 10	1.70162
24 24	617.43850	24 20 5	8.01704	14 14 6 6	-2.98394	21 21 11 10	0.66161
		24 20 6	-8.60607	14 14 7 1	-0.51468	21 21 12 10	0.99494
I J K	F(I,J,K)	24 20 7	-15.76698	14 14 7 2	-1.62720	21 21 12 11	1.05469
		24 20 9	8.09309	14 14 7 3	-1.03494	21 21 12 12	-2.29459
1 1 1	-724.97613	24 21 1	3.73092	14 14 7 4	-8.29055	21 21 13 10	-1.08800
2 1 1	164.29504	24 21 2	-37.14058	14 14 7 5	2.45050	21 21 13 11	0.23881
2 2 1	-366.31056	24 21 3	-5.90870	14 14 7 6	2.00531	21 21 13 12	-1.72075
2 2 2	-668.59509	24 21 4	8.03485	14 14 7 7	12.30721	21 21 13 13	-4.61007
3 1 1	-54.82361	24 21 5	-13.88723	14 14 8 1	-2.24654	21 21 14 14	0.58856
3 2 1	47.22178	24 21 6	-5.21838	14 14 8 2	-0.43377	21 21 15 14	-0.27913
3 2 2	30.69760	24 21 7	-3.41360	14 14 8 3	-2.53699	21 21 15 15	-1.19020
3 3 1	85.95348	24 21 8	0.51960	14 14 8 4	0.69459	21 21 16 16	-5.42689
3 3 2	-42.10440	24 21 9	-6.99179	14 14 8 5	1.90846	21 21 17 17	-10.71181
3 3 3	-197.59620	24 22 1	-5.30262	14 14 8 6	1.35281	21 21 18 17	-6.41229
4 1 1	65.37882	24 22 2	-66.41314	14 14 8 7	-1.19337	21 21 18 18	-11.86169
4 2 1	-7.64113	24 22 3	2.18731	14 14 8 8	4.65928	21 21 19 17	1.30705
4 2 2	32.76299	24 22 4	-13.22123	14 14 9 1	0.16635	21 21 19 18	2.29402
4 3 1	4.02001	24 22 5	1.08635	14 14 9 2	-1.50139	21 21 19 19	-9.03230
4 3 2	3.70469	24 22 6	-5.07516	14 14 9 3	1.38228	21 21 20 17	1.01676
4 3 3	42.95127	24 22 7	3.23295	14 14 9 4	0.56330	21 21 20 18	1.01220
4 4 1	30.14508	24 22 8	9.22072	14 14 9 5	-1.83477	21 21 20 19	-3.54793
4 4 2	70.34999	24 22 9	6.47774	14 14 9 6	-0.29547	21 21 20 20	-4.02430
4 4 3	41.93148	24 23 1	-55.42792	14 14 9 7	-2.61984	21 21 21 17	-0.14370
4 4 4	6.14630	24 23 2	-17.80576	14 14 9 8	-3.60754	21 21 21 18	0.18866
5 1 1	28.54566	24 23 3	-2.70745	14 14 9 9	2.18893	21 21 21 20	1.16851
5 2 1	-19.18291	24 23 4	11.78751	14 14 10 10	52.76779	21 21 21 21	-0.47391
5 2 2	-0.30948	24 23 5	2.52232	14 14 11 10	3.57171	22 17 1 1	5.81538
5 3 1	-52.43809	24 23 6	-9.86953	14 14 11 11	44.24946	22 17 2 2	2.42136
5 3 2	22.42178	24 23 7	3.27725	14 14 12 10	27.22191	22 17 3 3	-2.04914
5 3 3	97.17213	24 23 8	-23.45241	14 14 12 11	28.02065	22 17 4 4	-0.94167
5 4 1	-10.65688	24 23 9	4.12693	14 14 12 12	42.07747	22 17 5 5	-0.53715
5 4 2	-31.39787	24 24 1	31.60195	14 14 13 10	-18.28204	22 17 6 6	-0.20201
5 4 3	-139.54208	24 24 2	34.11737	14 14 13 11	5.96774	22 17 7 7	-0.44162
5 4 4	-13.07176	24 24 3	16.66465	14 14 13 12	-13.98028	22 17 9 9	0.14298
5 5 1	34.39817	24 24 4	2.34358	14 14 13 13	16.07984	22 17 10 10	-0.52702
5 5 2	7.20286	24 24 5	-2.11857	14 14 14 14	59.40529	22 17 11 11	-1.09005
5 5 3	-47.62032	24 24 6	-4.00350	15 14 1 1	-69.26337	22 17 12 12	-0.19154
5 5 4	-182.03265	24 24 7	-1.23256	15 14 2 2	67.72613	22 17 14 14	-0.20836
5 5 5	119.34545	24 24 8	9.53367	15 14 3 3	2.56115	22 17 15 15	-1.34150
6 1 1	-58.74518			15 14 4 4	-3.73690	22 17 16 16	-0.26609
6 2 1	-3.46042	I J K L	F(I,J,K,L)	15 14 5 5	3.75429	22 17 17 17	3.28754
6 2 2	-55.36875			15 14 6 6	0.48371	22 18 1 1	-4.88698
6 3 1	-9.23755	1 1 1 1	221.10900	15 14 7 7	-12.92356	22 18 2 2	-2.01199
6 3 2	-6.17250	2 1 1 1	-70.63778	15 14 8 8	12.60044	22 18 3 3	0.50117
6 3 3	-145.55838	2 2 1 1	63.45086	15 14 9 9	5.35486	22 18 4 4	-2.42854
6 4 1	-15.20870	2 2 2 1	72.09114	15 14 10 10	15.66928	22 18 5 5	-0.88996
6 4 2	-10.04017	2 2 2 2	227.62475	15 14 11 11	16.96064	22 18 6 6	-0.91918
6 4 3	-50.73208	3 1 1 1	17.62710	15 14 12 12	-37.35749	22 18 7 7	0.09424
6 4 4	-126.90085	3 2 1 1	-10.02277	15 14 13 13	15.13446	22 18 8 8	0.71103
6 5 1	5.90251	3 2 2 1	-2.82271	15 14 14 14	-18.09998	22 18 9 9	0.41394
6 5 2	2.69032	3 2 2 2	-17.96908	15 15 1 1	-166.99584	22 18 10 10	0.65387
6 5 3	-14.23214	3 3 1 1	-11.30744	15 15 2 1	33.14236	22 18 11 11	2.28155
6 5 4	-9.51512	3 3 2 1	3.95946	15 15 2 2	-92.84654	22 18 12 12	-0.25707
6 5 5	-219.69675	3 3 2 2	-1.97113	15 15 3 1	-9.57866	22 18 13 13	1.34718
6 6 1	20.64851	3 3 3 1	-15.58786	15 15 3 2	8.24285	22 18 14 14	-0.39339
6 6 2	6.62924	3 3 3 2	5.12247	15 15 3 3	1.21029	22 18 15 15	2.85917
6 6 3	-13.90656	3 3 3 3	49.95161	15 15 4 1	11.88444	22 18 16 16	0.78633
6 6 4	-6.93321	4 1 1 1	-18.79577	15 15 4 2	-2.45653	22 18 17 17	-0.80317
6 6 5	-85.71001	4 2 1 1	5.13672	15 15 4 3	0.64775	22 18 18 17	2.46878
6 6 6	-144.20989	4 2 2 1	-6.43110	15 15 4 4	-0.55106	22 18 18 18	-3.80854
7 1 1	20.05726	4 2 2 2	-6.39681	15 15 5 1	5.11073	22 19 1 1	-3.95488
7 2 1	-9.61550	4 3 1 1	1.74509	15 15 5 2	-4.14905	22 19 2 2	25.35308
7 2 2	-3.08983	4 3 2 2	2.11328	15 15 5 3	-3.13825	22 19 3 3	0.11724

I	J	K	F(I,J,K)	I	J	K	L	F(I,J,K,L)	I	J	K	L	F(I,J,K,L)	I	J	K	L	F(I,J,K,L)
7	3	1	-11.45474	4	3	3	1	5.39362	15	15	5	5	-1.32873	22	19	4	4	-0.69708
7	3	2	12.88756	4	3	3	2	-1.96378	15	15	6	1	-10.70342	22	19	5	5	11.24074
7	3	3	53.09408	4	3	3	3	-5.76900	15	15	6	2	-1.11711	22	19	6	6	-1.02473
7	4	1	-21.99480	4	4	1	1	-3.95817	15	15	6	3	-1.96360	22	19	7	7	-10.86854
7	4	2	-71.63248	4	4	2	1	-11.08228	15	15	6	4	0.18656	22	19	8	8	2.55892
7	4	3	-6.52084	4	4	2	2	-30.66462	15	15	6	5	1.42176	22	19	9	9	0.74618
7	4	4	8.19511	4	4	3	1	2.76164	15	15	6	6	-0.68190	22	19	10	10	-0.47431
7	5	1	10.59619	4	4	3	2	3.86404	15	15	7	1	3.93914	22	19	11	11	-1.91380
7	5	2	2.73444	4	4	3	3	13.72771	15	15	7	3	-0.86367	22	19	12	12	-4.34689
7	5	3	-84.35144	4	4	4	1	1.15057	15	15	7	4	-6.57464	22	19	13	13	1.74050
7	5	4	-41.46769	4	4	4	2	4.00665	15	15	7	5	1.24275	22	19	14	14	-3.04401
7	5	5	-64.13324	4	4	4	3	8.58862	15	15	7	6	1.56295	22	19	15	15	-1.15679
7	6	1	-1.60469	4	4	4	4	5.90888	15	15	7	7	12.17885	22	19	16	16	-8.44054
7	6	2	5.92761	5	1	1	1	-7.88276	15	15	8	1	-1.66008	22	19	17	17	9.05533
7	6	3	-24.37001	5	2	1	1	3.53731	15	15	8	2	-0.22639	22	19	18	18	12.18959
7	6	4	-52.74863	5	2	2	1	-1.26635	15	15	8	3	-9.44367	22	19	19	17	-1.50186
7	6	5	-27.29258	5	2	2	2	1.10411	15	15	8	4	1.73615	22	19	19	18	-4.50252
7	6	6	-11.37125	5	3	1	1	5.70177	15	15	8	5	5.89798	22	19	19	19	5.98808
7	7	1	59.31469	5	3	3	1	8.17866	15	15	8	6	3.62658	22	20	1	1	20.93314
7	7	2	145.19418	5	3	3	2	-4.96214	15	15	8	7	2.10199	22	20	2	2	10.78879
7	7	3	-4.91192	5	3	3	3	-29.54815	15	15	8	8	24.62297	22	20	4	4	1.23805
7	7	4	-3.55712	5	4	1	1	-0.27061	15	15	9	1	1.17675	22	20	5	5	7.61090
7	7	5	-8.81431	5	4	2	2	2.44102	15	15	9	2	-1.83036	22	20	6	6	0.35018
7	7	6	-32.82692	5	4	3	3	2.73074	15	15	9	3	8.93607	22	20	7	7	-2.93359
7	7	7	-9.66546	5	4	4	1	-0.26656	15	15	9	4	0.50639	22	20	8	8	-6.51854
8	1	1	-3.08477	5	4	4	2	-0.37615	15	15	9	5	-5.75359	22	20	9	9	-4.93643
8	2	1	-1.46263	5	4	4	3	5.83886	15	15	9	6	-2.81775	22	20	10	10	-2.46640
8	2	2	-6.65092	5	4	4	4	-1.81064	15	15	9	7	-4.14397	22	20	11	11	-3.53821
8	3	1	-40.71898	5	5	1	1	-3.74966	15	15	9	8	-18.11875	22	20	12	12	-1.83290
8	3	2	18.68488	5	5	2	1	0.61851	15	15	9	9	10.65157	22	20	14	14	-2.95913
8	3	3	-53.88388	5	5	2	2	-2.26381	15	15	10	10	71.13966	22	20	15	15	-5.34974
8	4	1	8.02205	5	5	3	1	-5.07263	15	15	11	10	-49.89537	22	20	16	16	-6.79471
8	4	2	8.01324	5	5	3	2	3.01595	15	15	11	11	105.56268	22	20	17	17	16.91029
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8	4	4	31.56256	5	5	4	1	1.11341	15	15	12	11	17.77577	22	20	19	19	8.47305
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8	5	2	-8.39102	5	5	4	3	0.56567	15	15	13	10	-56.80544	22	20	20	18	-0.63553
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I J K	Fl(I,J,K)	I J K L	Fl(I,J,K,L)	I J K L	Fl(I,J,K,L)	I J K L	Fl(I,J,K,L)
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I	J	K	Fl(I,J,K)	I	J	K	L	Fl(I,J,,K,L)	I	J	K	L	Fl(I,J,K,L)	I	J	K	L	Fl(I,J,K,L)
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23	20	3	-40.13278	13	12	9	9	0.45912	21	19	12	12	-1.62439	24	24	9	3	1.31834
23	20	4	-16.45730	13	12	10	10	-9.89125	21	19	13	13	-0.38722	24	24	9	4	1.06156
23	20	5	4.10550	13	12	11	11	-10.42580	21	19	14	14	-1.60799	24	24	9	6	-0.90319
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23	20	7	-13.46277	13	12	12	11	-9.89993	21	19	17	17	4.78318	24	24	9	8	-3.46593
23	20	8	-10.01601	13	12	12	12	-9.69662	21	19	18	18	6.48403	24	24	9	9	3.25112
23	20	9	-14.02407	13	13	1	1	-43.21697	21	19	19	17	-1.22985	24	24	10	10	0.42088
23	21	1	-16.63294	13	13	2	1	13.40812	21	19	19	18	-0.71097	24	24	11	10	-0.54908
23	21	2	32.73730	13	13	2	2	-13.58271	21	19	19	19	5.84370	24	24	11	11	2.31098
23	21	3	11.40578	13	13	3	1	1.12578	21	20	1	1	11.04812	24	24	12	10	3.45376
23	21	4	4.72723	13	13	3	2	-2.39791	21	20	2	2	6.42311	24	24	12	11	2.70910
23	21	5	1.54838	13	13	3	3	-29.55921	21	20	3	3	-0.88058	24	24	12	12	2.07918
23	21	7	-3.05065	13	13	4	1	0.32147	21	20	4	4	6.24904	24	24	13	10	-3.31468
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23	21	9	-7.30825	13	13	4	3	-3.87258	21	20	6	6	0.82712	24	24	13	13	4.19674
23	22	1	-31.20773	13	13	4	4	-16.66251	21	20	7	7	0.82759	24	24	14	14	2.78393
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23	22	3	-4.06965	13	13	5	2	0.95157	21	20	9	9	-1.09898	24	24	15	15	5.91724
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23	23	3	21.62158	13	13	6	6	-14.29872	21	20	19	19	2.21417	24	24	20	18	-0.23549
23	23	4	27.97548	13	13	7	2	0.96567	21	20	20	17	2.47734	24	24	20	20	-0.19959
23	23	5	-14.31672	13	13	7	4	-4.16445	21	20	20	18	0.81889	24	24	21	17	0.29431
23	23	6	-24.63568	13	13	7	5	-8.34051	21	20	20	19	1.71943	24	24	21	20	-1.09675
23	23	7	26.70420	13	13	7	6	-1.87223	21	20	20	20	-6.10254	24	24	21	21	-1.39372
23	23	8	7.87544	13	13	7	7	-4.89016	21	21	1	1	-6.83154	24	24	22	19	-2.98719
23	23	9	6.26367	13	13	8	1	0.40636	21	21	2	1	-3.98065	24	24	22	20	-1.35844
24	14	10	4.02255	13	13	8	2	-0.50242	21	21	2	2	-16.17133	24	24	22	21	5.38399
24	14	11	1.82994	13	13	8	3	-7.21442	21	21	3	1	0.58939	24	24	22	22	5.92106
24	14	12	-1.32755	13	13	8	4	1.61621	21	21	3	2	-1.24624	24	24	23	17	0.27193
24	14	13	-3.82617	13	13	8	5	6.63318	21	21	3	3	-6.21524	24	24	23	18	0.33239
24	15	10	5.66165	13	13	8	7	2.59712	21	21	4	1	0.26925	24	24	23	19	-2.66839
24	15	11	4.22400	13	13	8	8	-2.06119	21	21	4	2	1.93766	24	24	23	20	1.49655
24	15	13	8.83905	13	13	9	1	1.08908	21	21	4	3	0.42974	24	24	23	21	1.15374
24	16	10	-4.35392	13	13	9	3	0.86090	21	21	4	4	-3.71206	24	24	23	22	2.35497
24	16	11	-4.09128	13	13	9	4	-0.56706	21	21	5	1	-1.04522	24	24	23	23	6.61480
24	16	12	2.08795	13	13	9	5	1.15440	21	21	5	2	-2.28064	24	24	24	17	-0.34254
24	16	13	11.05833	13	13	9	8	-4.61107	21	21	5	3	-1.69959	24	24	24	18	0.58225
24	17	1	-6.62970	13	13	9	9	-2.25039	21	21	5	4	4.07812	24	24	24	19	3.19530
24	17	2	3.73772	13	13	10	10	30.91093	21	21	5	5	-11.70426	24	24	24	20	0.55743
24	17	3	8.77105	13	13	11	10	-18.74849	21	21	6	1	0.37279	24	24	24	21	-1.88207
24	17	4	39.14348	13	13	11	11	27.51931	21	21	6	3	-0.24388	24	24	24	22	-3.79789
24	17	5	-10.76076	13	13	12	10	3.10070	21	21	6	4	-0.61636	24	24	24	23	-4.63628
24	17	6	-10.62285	13	13	12	11	-1.09967	21	21	6	5	-0.89907	24	24	24	24	8.06705
24	17	7	-57.94551	13	13	12	12	7.53907	21	21	6	6	-1.05654					
24	17	8	-39.58356	13	13	13	10	-9.23371	21	21	7	1	-0.57940					

Table S38: The quartic potential energy surface of Pyrazine. The calculation was done by using B3LYP/6-311++G(2d,2p) method. The force constant (FIs) are in cm⁻¹ units.

I J	F(I,J)	I J K	FI(I,J,K)	I J K L	F(I,I,J,K,L)	I J K L	FI(I,J,K,L)
1 1	3176.08814	23 20 6	-19.48348	14 13 5 5	1.95702	20 20 5 3	4.30058
2 2	1612.14157	23 20 7	16.77279	14 13 6 6	41.28632	20 20 5 4	5.42038
3 3	1253.07407	23 21 6	6.62780	14 13 7 7	17.16455	20 20 5 5	-10.04325
4 4	1038.99428	23 21 7	21.16995	14 13 8 8	45.04839	20 20 6 6	-2.83726
5 5	615.06995	23 22 6	-7.36216	14 13 9 9	-52.31181	20 20 7 6	4.26708
6 6	1005.85091	23 22 7	20.88517	14 13 10 10	5.57994	20 20 7 7	-11.81120
7 7	351.46148	23 23 1	521.71065	14 13 11 11	2.66530	20 20 8 8	-1.49770
8 8	944.94234	23 23 2	-7.16690	14 13 13 13	43.81198	20 20 9 9	-17.77247
9 9	3156.26226	23 23 3	11.60115	14 14 1 1	-16.13637	20 20 10 9	3.17624
10 10	1518.68368	23 23 4	-9.29001	14 14 2 1	-0.28175	20 20 10 10	17.89902
11 11	1164.79526	23 23 5	-8.36496	14 14 2 2	-11.42264	20 20 11 9	-2.29489
12 12	1037.75285	24 13 9	-68.66218	14 14 3 1	0.72942	20 20 11 10	11.10921
13 13	993.16846	24 13 10	39.37224	14 14 3 2	-6.10386	20 20 11 11	14.22026
14 14	778.39961	24 13 11	-16.02030	14 14 3 3	-4.80632	20 20 12 9	-2.38698
15 15	3170.19334	24 13 12	10.84001	14 14 4 1	-0.73503	20 20 12 10	9.27190
16 16	1445.53416	24 14 9	-16.12906	14 14 4 3	-1.88047	20 20 12 11	16.00858
17 17	1208.13429	24 14 10	-22.12704	14 14 4 4	-5.28124	20 20 12 12	0.26102
18 18	1089.51389	24 14 11	-40.11031	14 14 5 1	-0.32784	20 20 13 13	-3.28044
19 19	3155.11452	24 14 12	-17.23457	14 14 5 2	0.64339	20 20 14 13	4.47155
20 20	1575.70792	24 15 8	-68.61270	14 14 5 3	1.86799	20 20 14 14	-15.15166
21 21	1378.75825	24 16 8	-31.19556	14 14 5 4	-0.84639	20 20 15 15	-17.93490
22 22	720.69536	24 17 8	-58.37750	14 14 5 5	-1.12287	20 20 16 15	-2.46734
23 23	803.60623	24 18 8	9.18427	14 14 6 6	7.48895	20 20 16 16	0.35483
24 24	433.76816	24 19 6	-65.40121	14 14 7 6	5.45743	20 20 17 15	-0.29495
		24 19 7	-51.33849	14 14 7 7	10.05052	20 20 17 16	-6.94495
		24 20 6	22.20977	14 14 8 8	10.74726	20 20 17 17	50.94295
		24 20 7	-66.54924	14 14 9 9	-16.28887	20 20 18 15	5.49530
1 1 1	-972.81427	24 21 6	23.39504	14 14 10 9	0.65566	20 20 18 16	-7.46684
2 1 1	-44.11559	24 21 7	47.89546	14 14 10 10	-4.74450	20 20 18 17	-8.49421
2 2 1	91.14069	24 22 6	-2.89596	14 14 11 9	-0.21131	20 20 18 18	-4.01639
2 2 2	-120.60160	24 22 7	3.63596	14 14 11 10	-4.21339	20 20 19 19	-17.73418
3 1 1	10.79162	24 23 1	-76.18715	14 14 11 11	-6.23406	20 20 20 19	3.28421
3 2 1	-79.38117	24 23 2	-57.13303	14 14 12 9	0.39203	20 20 20 20	32.03686
3 2 2	-25.80729	24 23 3	29.18663	14 14 12 10	-2.65578	21 19 1 1	-4.15204
3 3 1	121.58611	24 23 4	-13.20787	14 14 12 11	-1.85927	21 19 2 2	3.23488
3 3 2	-9.67520	24 23 5	-9.54679	14 14 12 12	-2.95379	21 19 3 3	-0.79773
3 3 3	18.09526	24 24 1	11.71838	14 14 13 13	9.89366	21 19 4 4	0.43629
4 1 1	20.47227	24 24 2	-55.06642	14 14 14 13	3.83195	21 19 6 6	0.35371
4 2 1	22.30109	24 24 3	-51.20560	14 14 14 14	-2.54513	21 19 7 7	-1.72733
4 2 2	157.72882	24 24 4	-65.01077	15 15 1 1	273.28203	21 19 8 8	-3.32329
4 3 1	-44.78281			15 15 2 1	13.48138	21 19 9 9	-1.35609
4 3 2	71.38025	I J K L	FI(I,J,K,L)	15 15 2 2	-41.64195	21 19 10 10	3.32102
4 3 3	64.84062			15 15 3 1	-7.88595	21 19 11 11	-6.56294
4 4 1	25.39190	1 1 1 1	273.15460	15 15 3 2	54.22245	21 19 12 12	1.58527
4 4 2	-15.34264	2 1 1 1	13.74651	15 15 3 3	-73.79494	21 19 13 13	-0.22155
4 4 3	10.24601	2 2 1 1	-40.80870	15 15 4 1	-4.45432	21 19 14 14	0.38874
4 4 4	113.73222	2 2 2 1	-7.12377	15 15 4 2	-18.27359	21 19 15 15	-4.10149
5 1 1	-7.31528	2 2 2 2	23.92325	15 15 4 3	23.57784	21 19 16 16	-1.55188
5 2 1	-70.50828	3 1 1 1	-7.70337	15 15 4 4	-7.89114	21 19 17 17	2.12354
5 2 2	5.88404	3 2 1 1	53.87357	15 15 5 1	-0.74439	21 19 18 18	2.66860
5 3 1	82.14521	3 2 2 1	2.10767	15 15 5 2	26.94659	21 19 19 19	-1.75740
5 3 2	8.56263	3 2 2 2	5.13270	15 15 5 3	-38.26923	21 20 1 1	-40.01613
5 3 3	-22.13599	3 3 1 1	-73.48516	15 15 5 4	12.02671	21 20 2 2	-0.39091
5 4 1	-27.00550	3 3 2 1	-2.04192	15 15 5 5	-20.65455	21 20 3 3	5.96146
5 4 2	-23.34487	3 3 2 2	13.87224	15 15 6 6	-157.83614	21 20 4 4	-2.01350
5 4 3	-7.70907	3 3 3 1	-0.30592	15 15 7 6	-115.09731	21 20 5 5	5.67650
5 4 4	16.00177	3 3 3 2	-12.94007	15 15 7 7	-83.29531	21 20 6 6	8.73006
5 5 1	48.97152	3 3 3 3	26.87884	15 15 8 8	-193.27529	21 20 7 7	6.49546
5 5 2	-33.29003	4 1 1 1	-4.23008	15 15 9 9	275.78554	21 20 8 8	11.64828
5 5 3	-15.80014	4 2 1 1	-17.84032	15 15 10 9	-2.85381	21 20 9 9	-40.66037
5 5 4	4.92275	4 2 2 1	1.49034	15 15 10 10	-79.75734	21 20 10 10	5.34476
5 5 5	-6.43581	4 2 2 2	-13.81484	15 15 11 9	4.18535	21 20 11 11	1.23235
6 6 1	322.07797	4 3 1 1	23.40568	15 15 11 10	54.57054	21 20 12 12	-0.16149
6 6 2	-16.32624	4 3 2 2	-6.77347	15 15 11 11	-39.52407	21 20 13 13	9.77511
6 6 3	-15.63272	4 3 3 1	-0.16229	15 15 12 9	-0.62585	21 20 14 14	4.63577
6 6 4	16.81824	4 3 3 2	4.61467	15 15 12 10	26.32739	21 20 15 15	-40.23578
6 6 5	-6.44769	4 3 3 3	-8.69546	15 15 12 11	-18.21128	21 20 16 16	10.76250
7 6 1	269.87962	4 4 1 1	-7.60275	15 15 12 12	-10.84916	21 20 17 17	-14.82450
7 6 2	-40.42033	4 4 2 1	-1.49312	15 15 13 13	-174.64800	21 20 18 18	7.83967
7 6 3	-8.19311	4 4 2 2	18.01036	15 15 14 13	-51.93848	21 20 19 19	-40.49812
7 6 4	17.72391	4 4 3 1	-0.34004	15 15 14 14	-16.27988	21 20 20 19	4.12675
7 6 5	-14.60285	4 4 3 2	6.43905	15 15 15 15	274.08888	21 20 20 20	-7.07319
7 7 1	201.68004	4 4 3 3	8.91781	16 15 1 1	14.14503	21 21 1 1	-103.95641
7 7 2	45.41130	4 4 4 1	1.61035	16 15 2 2	-6.38411	21 21 2 1	-0.28025
7 7 3	3.29729	4 4 4 2	-1.87125	16 15 3 3	0.27279	21 21 2 2	14.26617
7 7 4	-77.09342	4 4 4 3	-1.05254	16 15 4 4	-1.27207	21 21 3 1	-2.00311
7 7 5	-36.50116	4 4 4 4	11.18177	16 15 5 5	-0.62537	21 21 3 2	-19.45059
8 8 1	409.08564	5 1 1 1	-0.22903	16 15 6 6	-2.82755	21 21 3 3	26.12929
8 8 2	2.04248	5 2 1 1	27.28959	16 15 8 8	-2.84167	21 21 4 1	-1.66619
8 8 3	16.76819	5 2 2 1	1.92784	16 15 9 9	11.85053	21 21 4 2	7.16097
8 8 4	0.46110	5 2 2 2	-16.36779	16 15 10 10	-3.27323	21 21 4 3	-6.20207
8 8 5	15.36755	5 3 1 1	-38.36622	16 15 11 11	5.26284	21 21 4 4	3.14197
9 8 6	365.31974	5 3 2 2	1.94877	16 15 12 12	-1.05932	21 21 5 1	0.58788
9 8 7	285.72674	5 3 3 1	1.58128	16 15 13 13	-2.66789	21 21 5 2	-12.44088
9 9 1	-985.00206	5 3 3 2	-11.69248	16 15 14 14	-0.56504	21 21 5 3	15.69885
9 9 2	-40.95226	5 3 3 3	13.23101	16 15 15 15	14.25568	21 21 5 4	-4.76275

Table S39: The quartic potential energy surface pyrazine-d4. The calculation was done by using B3LYP/6-311++G(2d,2p) method. The force constants (FI) are in cm^{-1} units.

I	J	FI(I,J)	I	J	K	FI(I,J,K)	I	J	K	L	FI(I,J,K,L)	I	J	K	L	I(I,J,K,L)	
			23	21	7	24.52286	14	13	8	8	-38.67946	20	20	5	4	0.88128	
			23	22	6	3.57520	14	13	9	9	48.39149	20	20	5	5	-10.93266	
1	1	2357.91409	23	22	7	23.08771	14	13	10	10	-5.00726	20	20	6	6	-5.13485	
2	2	1569.25300	23	23	1	295.24364	14	13	11	11	0.19139	20	20	7	6	-3.75473	
3	3	1028.76951	23	23	2	-13.02019	14	13	12	12	-7.39333	20	20	7	7	-10.58360	
4	4	899.05689	23	23	3	20.24266	14	13	13	13	-15.99044	20	20	8	8	-4.69362	
5	5	599.50737	23	23	4	30.61644	14	14	1	1	-58.53346	20	20	9	9	-4.82455	
6	6	847.41849	23	23	5	-3.36970	14	14	2	1	-4.60869	20	20	10	9	-3.95841	
7	7	295.09026	24	13	9	68.79073	14	14	2	2	-2.30865	20	20	10	10	29.67068	
8	8	737.61681	24	13	10	-39.70192	14	14	3	1	-4.29317	20	20	11	9	-2.18407	
9	9	2333.73628	24	13	11	-8.22024	14	14	3	2	2.76870	20	20	11	10	2.86775	
10	10	1384.45684	24	13	12	4.13529	14	14	3	3	-2.61679	20	20	11	11	-9.25028	
11	11	1039.25169	24	14	9	-71.86686	14	14	4	1	1.15034	20	20	12	9	1.66702	
12	12	884.91047	24	14	10	-19.70409	14	14	4	2	-2.19676	20	20	12	10	-15.00334	
13	13	862.59377	24	14	11	16.70082	14	14	4	3	-0.47130	20	20	12	11	1.51315	
14	14	657.19486	24	14	12	30.05227	14	14	4	4	3.01674	20	20	12	12	9.06318	
15	15	2345.84941	24	15	8	-96.59902	14	14	5	1	-0.66516	20	20	13	13	-11.92983	
16	16	1289.82853	24	16	8	-21.04530	14	14	5	2	-2.87953	20	20	14	13	-6.92212	
17	17	1207.79534	24	17	8	-58.47415	14	14	5	3	-1.78899	20	20	14	14	-8.38449	
18	18	846.46297	24	18	8	10.48043	14	14	5	4	5.82331	20	20	15	15	-5.71454	
19	19	2325.09840	24	19	6	83.98003	14	14	5	5	2.57770	20	20	16	15	2.46404	
20	20	1558.02069	24	19	7	-79.97363	14	14	6	6	33.06683	20	20	16	16	-6.53522	
21	21	1047.81047	24	20	6	-28.49428	14	14	7	6	-31.75455	20	20	17	15	3.24888	
22	22	696.41327	24	20	7	-69.14411	14	14	7	7	32.93721	20	20	17	16	-7.51615	
23	23	609.96332	24	21	6	-13.23015	14	14	8	8	44.90608	20	20	17	17	55.25736	
24	24	414.27386	24	21	7	27.25561	14	14	9	9	-59.80369	20	20	18	15	0.96865	
			24	22	6	3.83590	14	14	10	9	-1.69046	20	20	18	16	-4.32033	
			24	22	7	-3.66650	14	14	10	10	-2.95674	20	20	18	17	-3.62376	
			24	23	1	-106.06212	14	14	11	9	3.55429	20	20	18	18	-1.01724	
			24	23	2	-58.11331	14	14	11	10	0.57924	20	20	19	19	-5.07518	
			24	23	3	5.16553	14	14	11	11	-3.88298	20	20	20	19	-2.17152	
			24	23	4	25.93578	14	14	12	9	0.62977	20	20	20	20	36.44918	
			24	23	5	-4.22044	14	14	12	10	5.16868	21	19	1	1	-4.11431	
			24	24	1	34.29128	14	14	12	11	0.92677	21	19	2	2	5.06553	
			24	24	2	-43.43585	14	14	12	12	4.19595	21	19	3	3	1.27337	
			24	24	3	71.65288	14	14	13	13	20.53300	21	19	4	4	0.27537	
			24	24	4	-5.61286	14	14	14	13	-24.25994	21	19	5	5	-0.53003	
			24	24	5	3.03685	14	14	14	14	27.47757	21	19	6	6	0.78569	
							15	15	1	1	142.43701	21	19	7	7	-1.24711	
							15	15	2	1	15.45486	21	19	8	8	-1.66965	
							15	15	2	2	-9.08585	21	19	9	9	0.71265	
			1	1	1	1	141.64946	15	15	3	1	14.96383	21	19	10	10	-0.70858
			2	1	1	1	15.81022	15	15	3	2	-4.51303	21	19	11	11	0.62265
			2	2	1	1	-8.33258	15	15	3	3	-3.02279	21	19	12	12	-1.00885
			2	2	2	1	-9.54900	15	15	4	1	-4.38518	21	19	14	14	0.83144
			2	2	2	2	27.69174	15	15	4	2	22.31162	21	19	15	15	-3.77362
			3	1	1	1	14.75118	15	15	4	3	13.48106	21	19	16	16	3.74360
			3	2	1	1	-4.50212	15	15	4	4	-40.58684	21	19	17	17	1.52300
			3	2	2	1	-6.88591	15	15	5	1	-0.75181	21	19	18	18	0.29957
			3	2	2	2	9.16825	15	15	5	2	13.93534	21	19	19	19	0.30753
			3	3	1	1	-2.82363	15	15	5	3	9.15134	21	20	1	1	-14.75644
			3	3	2	1	-1.52311	15	15	5	4	-28.44697	21	20	2	2	-4.63479
			3	3	2	2	13.56224	15	15	5	5	-20.93969	21	20	3	3	-1.97251
			3	3	3	1	-1.90091	15	15	6	6	-65.76376	21	20	4	4	2.67501
			3	3	3	2	-4.67719	15	15	7	6	63.88241	21	20	5	5	2.59987
			3	3	3	3	8.74058	15	15	7	7	-62.65492	21	20	6	6	1.89745
			4	1	1	1	-4.69510	15	15	8	8	-94.81222	21	20	7	7	2.92480
			4	2	1	1	21.80665	15	15	9	9	145.24147	21	20	8	8	3.57798
			4	2	2	1	-0.42253	15	15	10	9	6.83758	21	20	9	9	-14.81516
			4	2	2	2	15.31829	15	15	10	10	-18.54147	21	20	10	10	-3.26243
			4	3	1	1	13.45546	15	15	11	9	-11.25496	21	20	11	11	-0.85877
			4	3	2	2	7.35233	15	15	11	10	-6.56622	21	20	12	12	2.89434
			4	3	3	1	0.27847	15	15	11	11	-3.70016	21	20	13	13	1.90664
			4	3	3	2	1.44380	15	15	12	9	-3.90909	21	20	14	14	3.19519
			4	3	3	3	1.71718	15	15	12	10	-28.98335	21	20	15	15	-14.87886
			4	4	1	1	-39.85812	15	15	12	11	-10.40580	21	20	16	16	0.90895
			4	4	2	1	-5.17253	15	15	12	12	-48.15445	21	20	17	17	-6.33905
			4	4	2	2	7.71111	15	15	13	13	-39.69335	21	20	18	18	4.67906
			4	4	3	1	-2.94272	15	15	14	13	47.73786	21	20	19	19	-14.83834
			4	4	3	2	4.29318	15	15	14	14	-59.18050	21	20	20	20	-0.48954
			4	4	3	3	2.48243	15	15	15	15	143.56014	21	20	20	20	-2.80401
			4	4	4	1	-1.51650	16	15	1	1	19.72021	21	21	1	1	-56.50261
			4	4	4	2	-0.63480	16	15	2	2	-10.99606	21	21	2	1	-3.50881
			4	4	4	3	-1.72044	16	15	3	3	-1.84834	21	21	2	2	1.93906
			4	4	4	4	14.83711	16	15	4	4	-4.51305	21	21	3	1	-2.17350

I	J	K	FI(I,J,K)	I	J	K	L	FI(I,J,K,L)	I	J	K	L	FI(I,J,K,L)	I	J	K	L	I(I,J,K,L)
22	17	11	-14.45143	12	12	11	9	1.10943	19	19	14	13	48.53818	24	24	5	1	-0.33130
22	17	12	7.35642	12	12	11	10	-1.17857	19	19	14	14	-60.20061	24	24	5	2	1.16330
22	18	9	-29.44370	12	12	11	11	0.48256	19	19	15	15	145.80071	24	24	5	3	-0.45128
22	18	10	8.21013	12	12	12	9	-0.20542	19	19	16	15	18.18317	24	24	5	4	0.82211
22	18	11	4.14708	12	12	12	10	8.14884	19	19	16	16	-14.82146	24	24	5	5	5.06639
22	18	12	-27.02481	12	12	12	11	5.07644	19	19	17	15	3.09860	24	24	6	6	9.89257
22	19	1	-18.40740	12	12	12	12	13.50020	19	19	17	16	-8.54803	24	24	7	6	-3.93386
22	19	2	5.05368	13	13	1	1	-39.43963	19	19	17	17	-6.41044	24	24	7	7	26.81791
22	19	3	-0.36768	13	13	2	1	-0.13404	19	19	18	15	0.73454	24	24	8	8	11.72876
22	19	4	-23.74021	13	13	2	2	-13.09876	19	19	18	16	28.94463	24	24	9	9	-15.07900
22	19	5	-14.96580	13	13	3	1	-1.11837	19	19	18	17	15.91018	24	24	10	9	2.38939
22	20	1	-18.70669	13	13	3	3	-3.98518	19	19	18	18	-55.11123	24	24	10	10	-16.14134
22	20	2	-15.53739	13	13	4	1	1.45954	19	19	19	19	148.61467	24	24	11	9	1.03680
22	20	3	29.06214	13	13	4	2	-5.27979	20	19	1	1	6.74665	24	24	11	11	-5.23997
22	20	4	10.06870	13	13	4	3	-2.68355	20	19	3	3	-0.74311	24	24	12	10	6.59022
22	20	5	9.96167	13	13	4	4	1.81870	20	19	4	4	1.06390	24	24	12	11	-1.57460
22	21	1	-24.81550	13	13	5	1	-0.73199	20	19	5	5	0.21128	24	24	12	12	-5.74002
22	21	2	1.51536	13	13	5	2	-0.25998	20	19	7	7	-3.86523	24	24	13	13	10.04145
22	21	3	2.21469	13	13	5	3	-0.73652	20	19	8	8	-1.09767	24	24	14	13	-3.42510
22	21	4	-20.24665	13	13	5	4	3.55038	20	19	9	9	8.10604	24	24	14	14	13.02761
22	21	5	-5.57638	13	13	5	5	2.07620	20	19	10	10	-3.85962	24	24	15	15	-14.33680
22	22	1	4.17197	13	13	6	6	17.82203	20	19	11	11	2.06531	24	24	16	15	-2.09488
22	22	2	21.51739	13	13	7	6	-19.18097	20	19	12	12	-1.31933	24	24	16	16	-5.80873
22	22	3	-18.18095	13	13	7	7	29.91764	20	19	13	13	0.56116	24	24	17	15	-3.09714
22	22	4	-10.59154	13	13	8	8	31.06205	20	19	14	14	-0.55092	24	24	17	16	3.86523
22	22	5	-4.81198	13	13	9	9	-39.99637	20	19	15	15	7.11275	24	24	17	17	-34.24431
23	13	9	-166.26646	13	13	10	9	-0.28948	20	19	16	16	3.68196	24	24	18	15	0.27289
23	13	10	-19.06209	13	13	10	10	-5.52752	20	19	17	17	-4.75363	24	24	18	16	2.26736
23	13	11	-19.27378	13	13	11	9	0.90656	20	19	18	18	0.77743	24	24	18	17	4.46929
23	13	12	3.70852	13	13	11	10	0.91689	20	19	19	19	8.14045	24	24	19	19	-15.13901
23	14	9	203.54058	13	13	11	11	-0.44721	20	20	1	1	-5.66278	24	24	20	19	2.05644
23	14	10	2.18386	13	13	12	9	-0.17609	20	20	2	1	4.16112	24	24	20	20	-29.42542
23	14	11	-13.47754	13	13	12	10	4.74705	20	20	2	2	14.58912	24	24	21	19	1.23967
23	14	12	5.88223	13	13	12	11	1.18153	20	20	3	1	-0.30341	24	24	21	20	4.47931
23	15	8	260.11843	13	13	12	12	3.90371	20	20	3	2	-21.52545	24	24	21	21	-4.18600
23	16	8	15.98491	13	13	13	13	7.78989	20	20	3	3	16.90264	24	24	22	19	-0.81735
23	17	8	-6.17684	14	13	1	1	47.16597	20	20	4	1	0.15070	24	24	22	20	2.73959
23	18	8	20.66538	14	13	2	2	-6.85761	20	20	4	2	-4.38465	24	24	22	22	-3.01834
23	19	6	-211.15466	14	13	3	3	-2.63622	20	20	4	3	1.96185	24	24	23	23	25.97708
23	19	7	224.73139	14	13	4	4	-4.70200	20	20	4	4	0.28459	24	24	24	23	3.76137
23	20	6	-4.83654	14	13	5	5	-2.91491	20	20	5	1	1.99876	24	24	24	24	27.89250
23	20	7	6.41595	14	13	6	6	-26.28334	20	20	5	2	-1.24466					
23	21	6	-2.38144	14	13	7	7	-24.92315	20	20	5	3	-6.31497					

Table S40: The quartic potential energy surface of trans-butadiene. The calculation was done by using B3LYP/6-311++G(2d,2p) method. The force constants (F) are in cm^{-1} units.

I J	F(I,J)	I J K	F(I,J,K)	I J K L	F(I,J,K,L)	I J K L	F(I,J,K,L)
1 1	3225.98254	24 19 3	-5.24711	14 14 5 4	-3.62595	21 21 9 3	0.15120
2 2	3141.90745	24 19 4	0.77143	14 14 5 5	6.78011	21 21 9 4	-2.97915
3 3	3130.46038	24 19 5	12.23770	14 14 6 1	1.32551	21 21 9 5	-3.98999
4 4	1698.03059	24 19 6	-64.89978	14 14 6 2	-1.19051	21 21 9 6	-6.25342
5 5	1481.67652	24 19 7	-137.48299	14 14 6 3	1.00909	21 21 9 7	-12.46242
6 6	1319.61569	24 19 8	-259.80385	14 14 6 4	-9.09158	21 21 9 8	-24.94330
7 7	1229.76970	24 19 9	190.37166	14 14 6 5	10.19904	21 21 9 9	20.26206
8 8	900.38825	24 20 1	139.83912	14 14 6 6	12.46500	21 21 10 10	4.07168
9 9	519.29333	24 20 2	-43.45662	14 14 7 1	0.80807	21 21 11 10	-1.23630
10 10	1053.01767	24 20 3	20.63271	14 14 7 2	-2.20334	21 21 11 11	11.43817
11 11	941.11783	24 20 4	-13.88883	14 14 7 3	8.61781	21 21 12 10	-1.00505
12 12	538.56044	24 20 5	11.88343	14 14 7 4	8.83813	21 21 12 11	6.07485
13 13	172.96269	24 20 6	8.00972	14 14 7 5	-6.01445	21 21 12 12	13.13462
14 14	1000.01373	24 20 7	29.05057	14 14 7 6	-11.41021	21 21 13 10	3.90589
15 15	940.26865	24 20 8	-36.78080	14 14 7 7	2.72089	21 21 13 11	-6.59501
16 16	779.06676	24 20 9	39.91059	14 14 8 1	1.37783	21 21 13 12	5.52628
17 17	3226.37012	24 21 1	-216.07886	14 14 8 2	1.57279	21 21 13 13	-20.77173
18 18	3143.17691	24 21 2	1.82407	14 14 8 3	-0.87498	21 21 14 14	4.94933
19 19	3139.30065	24 21 3	19.75537	14 14 8 4	4.69419	21 21 15 14	-1.52064
20 20	1647.74912	24 21 4	-12.92516	14 14 8 5	2.98774	21 21 15 15	10.59752
21 21	1420.50113	24 21 5	6.58836	14 14 8 6	-2.07964	21 21 16 14	-2.95836
22 22	1327.12304	24 21 6	8.14200	14 14 8 7	8.27943	21 21 16 15	5.51629
23 23	1010.35741	24 21 7	17.12388	14 14 8 8	5.18415	21 21 16 16	4.73114
24 24	298.89119	24 21 8	-4.70128	14 14 9 1	-0.59898	21 21 17 17	-88.90048
		24 21 9	5.40944	14 14 9 2	-2.89340	21 21 18 17	-3.97984
I J K	F(I,J,K)	24 22 1	1.02275	14 14 9 3	4.10360	21 21 18 18	-29.33556
		24 22 2	-136.78324	14 14 9 4	-4.67397	21 21 19 17	-14.78284
1 1 1	-447.64648	24 22 3	57.09075	14 14 9 6	4.58176	21 21 19 18	11.38734
2 1 1	-825.45920	24 22 4	-10.90575	14 14 9 7	-6.38409	21 21 19 19	-60.48102
2 2 1	177.24644	24 22 5	14.94690	14 14 9 8	-5.66208	21 21 20 17	0.94408
2 2 2	-850.86618	24 22 6	20.53248	14 14 9 9	4.03733	21 21 20 18	-0.19258
3 1 1	-414.75166	24 22 7	-37.96089	14 14 10 10	154.08680	21 21 20 19	4.94292
3 2 1	48.81379	24 22 8	6.65556	14 14 11 10	-18.67791	21 21 20 20	16.56159
3 2 2	-106.13806	24 23 1	36.61008	14 14 11 11	37.07682	21 21 21 17	-2.15346
3 3 1	-169.88421	24 23 2	225.29095	14 14 12 10	117.90158	21 21 21 18	3.86706
3 3 2	-620.81328	24 23 3	189.19223	14 14 12 11	23.51798	21 21 21 19	-9.34164
3 3 3	955.71629	24 23 4	2.66034	14 14 12 12	179.48694	21 21 21 20	-3.40692
4 1 1	-3.61733	24 23 5	-6.67293	14 14 13 10	93.37593	21 21 21 21	12.93971
4 2 1	9.20671	24 23 6	33.26188	14 14 13 11	-18.50078	22 17 1 1	1.08359
4 2 2	41.50309	24 23 7	-18.11779	14 14 13 12	74.66116	22 17 2 2	-4.45786
4 3 2	10.70516	24 23 9	3.29654	14 14 13 13	51.40996	22 17 3 3	-1.86941
4 3 3	15.66287	24 24 1	49.37554	14 14 14 14	165.62315	22 17 4 4	2.02534
4 4 1	10.99915	24 24 2	289.59924	15 14 1 1	41.67509	22 17 5 5	0.09926
4 4 2	86.05580	24 24 3	83.99705	15 14 2 2	-19.32572	22 17 6 6	1.36215
4 4 3	-52.02509	24 24 4	-129.60437	15 14 3 3	-32.84406	22 17 7 7	4.24742
4 4 4	205.59105	24 24 5	1.07344	15 14 4 4	3.00491	22 17 8 8	5.96729
5 1 1	-67.60583	24 24 6	-84.88294	15 14 5 5	-3.10032	22 17 9 9	0.11809
5 2 1	18.63506	24 24 7	19.24104	15 14 6 6	4.13203	22 17 10 10	1.00513
5 2 2	12.50317	24 24 8	34.73814	15 14 7 7	0.84002	22 17 11 11	4.36858
5 3 1	-1.01265	24 24 9	-17.40578	15 14 8 8	-3.10673	22 17 12 12	5.88056
5 3 2	1.05004			15 14 10 10	22.56327	22 17 13 13	-4.68095
5 3 3	18.02484	I J K L	F(I,J,K,L)	15 14 11 11	-12.56946	22 17 14 14	1.48461
5 4 1	9.31385			15 14 12 12	-17.61409	22 17 15 15	3.66157
5 4 2	27.40077	1 1 1 1	307.80492	15 14 13 13	17.88060	22 17 16 16	3.84914
5 4 3	83.14826	2 1 1 1	55.57858	15 14 14 14	12.49305	22 17 17 17	0.95018
5 4 4	13.45186	2 2 1 1	199.18791	15 15 1 1	-193.50009	22 18 1 1	1.77687
5 5 1	59.88642	2 2 2 1	-84.99526	15 15 2 1	65.33058	22 18 2 2	-2.00036
5 5 2	115.38253	2 2 2 2	222.07070	15 15 2 2	-181.90999	22 18 3 3	4.57082
5 5 3	5.80078	3 1 1 1	61.16926	15 15 3 1	8.61288	22 18 4 4	-0.04774
5 5 4	12.30285	3 2 1 1	95.41923	15 15 3 2	-72.58961	22 18 5 5	-1.32607
5 5 5	64.02627	3 2 2 1	-26.42811	15 15 3 3	-39.90277	22 18 6 6	8.25171
6 1 1	38.28655	3 2 2 2	48.50404	15 15 4 1	1.53765	22 18 7 7	-7.43767
6 2 1	6.74484	3 3 1 1	57.09388	15 15 4 2	-1.66798	22 18 8 8	0.99638
6 2 2	3.45811	3 3 2 1	22.48757	15 15 4 3	-0.07740	22 18 9 9	2.93810
6 3 1	3.21299	3 3 2 2	114.85122	15 15 4 4	-0.59962	22 18 10 10	1.42880
6 3 2	2.74476	3 3 3 1	-34.52216	15 15 5 1	2.10974	22 18 11 11	1.33768
6 3 3	4.88669	3 3 3 2	-153.04710	15 15 5 2	-11.62459	22 18 12 12	5.27527
6 4 1	29.04497	3 3 3 3	381.81783	15 15 5 3	-4.65535	22 18 13 13	-6.83897
6 4 2	-42.76768	4 1 1 1	-3.08016	15 15 5 4	8.46196	22 18 14 14	-0.82097
6 4 3	68.03712	4 2 1 1	-0.40901	15 15 5 5	12.75640	22 18 15 15	1.10946
6 4 4	130.01917	4 2 2 1	-0.28722	15 15 6 1	2.49826	22 18 16 16	0.32953
6 5 1	62.07047	4 2 2 2	-11.34334	15 15 6 2	2.14397	22 18 17 17	1.87343
6 5 2	-7.88711	4 3 1 1	-1.60028	15 15 6 3	1.41502	22 18 18 17	-0.99970
6 5 3	-77.58000	4 3 2 2	-3.13531	15 15 6 4	-5.34764	22 18 18 18	2.33511
6 5 4	-28.00253	4 3 3 1	-1.28674	15 15 6 5	-6.76873	22 19 1 1	-3.87335
6 5 5	-9.61142	4 3 3 2	-4.49473	15 15 6 6	5.85963	22 19 2 2	3.60046
6 6 1	-14.66756	4 3 3 3	3.01560	15 15 7 1	3.49909	22 19 3 3	3.55609
6 6 2	85.13914	4 4 1 1	-23.44903	15 15 7 2	-1.50823	22 19 4 4	1.91189
6 6 3	-86.20120	4 4 2 1	2.62478	15 15 7 3	0.12741	22 19 5 5	1.89925
6 6 4	42.99571	4 4 2 2	-22.81671	15 15 7 4	-1.19136	22 19 6 6	-1.92548
6 6 5	0.82573	4 4 3 1	3.22493	15 15 7 5	-4.05404	22 19 7 7	-4.85627
6 6 6	79.58741	4 4 3 2	9.44539	15 15 7 6	5.66613	22 19 8 8	-1.63956
7 1 1	9.45957	4 4 3 3	-41.13197	15 15 7 7	4.44702	22 19 9 9	1.43855
7 2 1	19.60859	4 4 4 1	0.78136	15 15 8 1	-0.34619	22 19 10 10	-0.67942
7 2 2	-13.24907	4 4 4 2	6.69692	15 15 8 2	-4.19512	22 19 11 11	0.09409
7 3 1	12.14127	4 4 4 3	-2.99113	15 15 8 3	-1.34835	22 19 12 12	-2.12243

I J K	F(I,J,K)	I J K L	F(I,J,K,L)	I J K L	F(I,J,K,L)	I J K L	F(I,J,K,L)
18 15 10	-112.22249	9 7 7 5	-1.88572	19 17 11 11	-1.79503	23 23 3 1	-5.17246
18 15 11	-143.00635	9 7 7 6	-1.28604	19 17 12 12	-45.80425	23 23 3 2	-15.38460
18 15 12	39.30227	9 7 7 7	-14.56503	19 17 13 13	41.85578	23 23 3 3	-83.41319
18 15 13	74.94294	9 8 1 1	73.39912	19 17 14 14	-11.84477	23 23 4 1	0.65178
18 16 10	-87.68857	9 8 2 2	59.71271	19 17 15 15	49.10215	23 23 4 2	7.41048
18 16 11	34.80370	9 8 3 3	19.32278	19 17 16 16	-68.43473	23 23 4 3	5.60433
18 16 12	-219.79081	9 8 4 4	-5.29598	19 17 17 17	83.90366	23 23 4 4	13.21534
18 16 13	-118.73604	9 8 5 5	-28.64065	19 18 1 1	-71.24583	23 23 5 1	4.90916
18 17 1	293.99897	9 8 6 6	-9.39577	19 18 2 2	-56.78650	23 23 5 2	13.30250
18 17 2	-100.64716	9 8 7 7	-3.05046	19 18 3 3	135.66130	23 23 5 3	3.16017
18 17 3	-196.52895	9 8 8 1	-2.63280	19 18 4 4	-9.10494	23 23 5 4	14.67121
18 17 4	-6.80664	9 8 8 2	0.28540	19 18 5 5	9.17336	23 23 5 5	46.76598
18 17 5	-16.84165	9 8 8 3	1.02982	19 18 6 6	-21.77557	23 23 6 1	7.28969
18 17 6	-1.12795	9 8 8 4	2.18552	19 18 7 7	-10.07843	23 23 6 2	-5.50169
18 17 7	-6.52366	9 8 8 5	-9.69486	19 18 8 8	29.84520	23 23 6 3	-2.26375
18 17 8	-5.19718	9 8 8 6	-14.54993	19 18 9 9	14.02174	23 23 6 4	-20.25102
18 17 9	4.72192	9 8 8 7	-29.33284	19 18 10 10	-69.59343	23 23 6 5	-3.47811
18 18 1	-22.88285	9 8 8 8	-38.21916	19 18 11 11	65.71263	23 23 6 6	32.65452
18 18 2	-636.90531	9 9 1 1	-49.10075	19 18 12 12	14.06225	23 23 7 1	9.05194
18 18 3	1016.05641	9 9 2 1	4.04665	19 18 13 13	6.93894	23 23 7 2	-4.34923
18 18 4	20.00323	9 9 2 2	-42.80104	19 18 14 14	-82.56481	23 23 7 3	4.32704
18 18 5	12.05395	9 9 3 1	-2.82467	19 18 15 15	73.25616	23 23 7 4	7.20241
18 18 6	-0.59218	9 9 3 2	-15.84727	19 18 16 16	16.65827	23 23 7 5	-5.32337
18 18 7	-11.12567	9 9 3 3	-15.89276	19 18 17 17	-69.67882	23 23 7 6	-9.51026
18 18 8	-12.37447	9 9 4 1	0.59175	19 18 18 17	-50.63237	23 23 7 7	24.12001
18 18 9	-18.02849	9 9 4 2	2.81890	19 18 18 18	136.73562	23 23 8 1	11.49001
19 14 10	-70.18129	9 9 4 3	-0.72213	19 19 1 1	223.66634	23 23 8 2	-1.94087
19 14 11	-27.58024	9 9 4 4	-1.89880	19 19 2 1	-50.86024	23 23 8 3	1.59259
19 14 12	-314.12397	9 9 5 1	1.55176	19 19 2 2	213.18748	23 23 8 4	3.80106
19 14 13	-92.37871	9 9 5 2	1.08343	19 19 3 1	-5.05746	23 23 8 5	6.33026
19 15 10	42.46358	9 9 5 3	2.39681	19 19 3 2	59.75325	23 23 8 6	9.68803
19 15 11	391.14440	9 9 5 4	12.78731	19 19 3 3	97.95664	23 23 8 7	35.64764
19 15 12	-97.63344	9 9 5 5	21.98373	19 19 4 1	-1.03325	23 23 8 8	73.68361
19 15 13	-255.49105	9 9 6 2	-1.06357	19 19 4 2	-11.12972	23 23 9 1	-5.34957
19 16 10	-188.12080	9 9 6 3	1.61662	19 19 4 3	-4.64787	23 23 9 2	0.98047
19 16 11	59.55010	9 9 6 4	-5.83361	19 19 4 4	-22.62021	23 23 9 3	0.09654
19 16 12	321.88944	9 9 6 5	-5.44243	19 19 5 1	-4.26940	23 23 9 4	-2.92137
19 16 13	26.88698	9 9 6 6	11.03140	19 19 5 2	-7.53693	23 23 9 5	0.47886
19 17 1	-873.86119	9 9 7 1	1.43639	19 19 5 3	-1.84226	23 23 9 6	-6.00135
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23	19	7	-64.36907	13	12	12	11	-116.32556	21	19	16	16	3.06695	24	24	8	3	0.30419
23	19	8	-212.31640	13	12	12	12	76.59186	21	19	17	17	13.75070	24	24	8	4	6.66548
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23	20	3	-39.76241	13	13	3	1	20.03246	21	19	19	19	-2.81406	24	24	8	8	76.73851
23	20	4	-0.99452	13	13	3	2	1.14166	21	20	1	1	63.30898	24	24	9	1	0.33750
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23	20	6	-15.95370	13	13	4	1	-1.95488	21	20	3	3	-6.49349	24	24	9	4	3.47580
23	20	7	-21.73864	13	13	4	2	-10.57139	21	20	4	4	18.87169	24	24	9	5	2.48718
23	20	8	-19.77593	13	13	4	3	1.36477	21	20	5	5	-9.57191	24	24	9	6	-12.86699
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23	23	4	-24.72998	13	13	8	4	9.66325	21	21	3	2	-15.38925	24	24	19	17	-4.78619
23	23	5	-55.30008	13	13	8	5	-12.01704	21	21	3	3	-33.21581	24	24	19	18	31.35104
23	23	6	30.35324	13	13	8	6	8.39802	21	21	4	1	-0.64092	24	24	19	19	-110.80249
23	23	8	-26.08456	13	13	8	7	-3.32081	21	21	4	2	-1.99228	24	24	20	17	-0.63507
23	23	9	0.47088	13	13	8	8	1.01952	21	21	4	3	-2.01100	24	24	20	18	-1.45817
24	14	10	11.47701	13	13	9	1	0.66144	21	21	4	4	13.55032	24	24	20	19	-5.00024
24	14	11	1.60616	13	13	9	2	2.23060	21	21	5	1	-1.93302	24	24	20	20	-5.77353
24	14	12	2.59242	13	13	9	4	11.22775	21	21	5	2	-8.74896	24	24	21	17	0.73575
24	14	13	13.16542	13	13	9	5	4.69488	21	21	5	3	-4.94036	24	24	21	18	-3.08637
24	15	11	-6.95351	13	13	9	6	1.32972	21	21	5	4	5.35323	24	24	21	19	0.73035
24	15	12	-3.32581	13	13	9	7	-3.94628	21	21	5	5	14.08433	24	24	21	20	-46.36658
24	16	10	1.34924	13	13	9	8	-10.44633	21	21	6	1	-0.20570	24	24	21	21	37.94520
24	16	12	-2.75356	13	13	9	9	2.79488	21	21	6	2	4.72973	24	24	22	18	-2.92883
24	16	13	-14.10795	13	13	10	10	49.32476	21	21	6	3	3.00581	24	24	22	19	-1.29826
24	17	1	-3.15313	13	13	11	10	24.11663	21	21	6	4	-0.23946	24	24	22	20	19.20423
24	17	2	-5.12849	13	13	11	11	79.57656	21	21	6	5	1.87650	24	24	22	21	3.97029
24	17	3	-1.39904	13	13	12	11	-51.15776	21	21	6	6	10.49884	24	24	22	22	22.71543
24	17	4	-89.29176	13	13	12	12	108.76342	21	21	7	1	-0.34472	24	24	23	18	-1.04069
24	17	5	-231.73973	13	13	13	10	-9.54863	21	21	7	2	1.60649	24	24	23	19	-0.55246
24	17	6	51.27842	13	13	13	11	-30.10282	21	21	7	3	1.55396	24	24	23	21	-1.80891
24	17	7	-5.85490	13	13	13	12	38.50043	21	21	7	4	3.41011	24	24	23	22	-17.80720
24	17	8	-53.86282	13	13	13	13	247.13859	21	21	7	5	-0.17057	24	24	23	23	94.63640
24	17	9	17.62404	14	14	1	1	-50.67300	21	21	7	6	-1.06549	24	24	24	17	1.01673
24	18	1	3.69565	14	14	2	1	-31.08992	21	21	7	7	6.95382	24	24	24	18	-3.50719
24	18	2	6.34188	14	14	2	2	-69.47987	21	21	8	1	-8.82880	24	24	24	19	-3.22282
24	18	3	-16.34552	14	14	3	1	10.51458	21	21	8	2	2.89831	24	24	24	20	-3.56961
24	18	4	-60.20190	14	14	3	2	87.22612	21	21	8	3	-0.09779	24	24	24	21	-3.90520
24	18	5	17.75505	14	14	3	3	-230.49909	21	21	8	4	0.79758	24	24	24	22	-45.54285
24	18	6	130.98577	14	14	4	1	-1.36732	21	21	8	5	7.47751	24	24	24	23	72.12210
24	18	7	-4.57184	14	14	4	2	-1.28810	21	21	8	6	6.00865	24	24	24	24	157.55111
24	18	8	65.04100	14	14	4	3	2.10407	21	21	8	7	15.96236					
24	18	9	-35.01239	14	14	4	4	4.23289	21	21	8	8	34.38544					
24	19	1	-4.18298	14	14	5	2	3.08322	21	21	9	1	8.03068					
24	19	2	2.74372	14	14	5	3	-2.50044	21	21	9	2	-3.28697					

Table S41: The quartic potential energy surface of trans-butadiene-d6. The calculation was done by using B3LYP/6-311++G(2d,2p) method. The force constants (F) are in cm^{-1} units.

I J	F(I,J)	I J K	F(I,J,K)	I J K L	F(I,J,K,L)	I J K L	F(I,J,K,L)
1 1	2403.19204	24 18 7	72.25110	14 14 3 3	-36.81387	21 21 8 8	16.27315
2 2	2326.05994	24 18 8	56.98892	14 14 4 1	0.39123	21 21 9 1	2.38542
3 3	2283.22822	24 18 9	-42.62547	14 14 4 2	-2.70771	21 21 9 2	2.71654
4 4	1632.66662	24 19 1	-8.01276	14 14 4 3	-2.88436	21 21 9 3	-2.61721
5 5	1209.77842	24 19 2	-4.67209	14 14 4 4	-13.53885	21 21 9 4	-4.13593
6 6	1068.71281	24 19 3	-1.00752	14 14 5 1	1.08047	21 21 9 5	-4.76940
7 7	940.59609	24 19 4	-1.12411	14 14 5 2	-1.50647	21 21 9 6	-2.70024
8 8	747.28761	24 19 5	-23.97655	14 14 5 3	-0.88080	21 21 9 7	4.56610
9 9	447.72921	24 19 6	53.00730	14 14 5 4	1.53242	21 21 9 8	-14.68215
10 10	792.09341	24 19 7	18.28131	14 14 5 5	-5.53215	21 21 9 9	14.03621
11 11	741.14370	24 19 8	-153.55940	14 14 6 1	-0.71268	21 21 10 10	7.37139
12 12	391.75812	24 19 9	155.65590	14 14 6 2	-0.89503	21 21 11 10	-1.15409
13 13	149.80407	24 20 1	-49.80648	14 14 6 4	-0.35981	21 21 11 11	3.17069
14 14	828.46073	24 20 2	-16.99913	14 14 6 5	3.67733	21 21 12 10	-2.28118
15 15	718.29648	24 20 3	2.10298	14 14 6 6	0.59009	21 21 12 11	8.50862
16 16	615.16107	24 20 4	17.51493	14 14 7 1	0.27545	21 21 12 12	11.74299
17 17	2403.08966	24 20 5	-27.67436	14 14 7 2	-0.24146	21 21 13 10	4.99417
18 18	2327.67118	24 20 6	15.51164	14 14 7 3	-1.57356	21 21 13 11	1.19554
19 19	2286.25090	24 20 7	19.31646	14 14 7 4	-6.73474	21 21 13 12	1.13198
20 20	1564.33426	24 20 8	30.62143	14 14 7 5	4.70556	21 21 13 13	-3.74472
21 21	1070.14285	24 20 9	-47.30788	14 14 7 6	1.13177	21 21 14 14	4.94172
22 22	1023.10351	24 21 1	-143.26057	14 14 7 7	6.29884	21 21 15 14	-0.20090
23 23	757.61651	24 21 2	54.74976	14 14 8 1	0.14163	21 21 15 15	4.78509
24 24	250.66703	24 21 3	-17.35035	14 14 8 2	-0.61897	21 21 16 14	4.14618
I J K	F(I,J,K)	24 21 4	-11.37138	14 14 8 3	0.23620	21 21 16 15	4.72675
1 1 1	-184.01824	24 21 5	3.10933	14 14 8 4	0.29748	21 21 16 16	5.90971
2 1 1	271.82762	24 21 6	3.45519	14 14 8 5	4.71438	21 21 17 17	-49.78694
3 1 1	6.97431	24 21 7	8.96733	14 14 8 6	-1.44444	21 21 18 17	9.70613
4 1 1	646.92102	24 21 8	5.54520	14 14 8 7	-1.95469	21 21 18 18	-35.21400
5 1 1	-543.52545	24 21 9	-6.89994	14 14 8 8	0.41736	21 21 19 17	-21.50613
6 1 1	-84.26575	24 22 1	-98.12986	14 14 9 2	0.25740	21 21 19 18	-6.22330
7 1 1	212.41107	24 22 2	-80.47580	14 14 9 4	-1.13768	21 21 19 19	-33.71973
8 1 1	-1.22363	24 22 3	46.31455	14 14 9 5	1.59427	21 21 20 17	3.27033
9 1 1	365.22716	24 22 4	4.90799	14 14 9 6	0.48077	21 21 20 18	-3.08936
10 1 1	-295.40914	24 22 5	1.52314	14 14 9 7	3.44018	21 21 20 19	1.65962
11 1 1	77.08404	24 22 6	-11.21598	14 14 9 8	-3.37145	21 21 20 20	-0.17305
12 1 1	-4.79334	24 22 7	-16.67610	14 14 9 9	2.59103	21 21 21 17	-2.01211
13 1 1	84.78026	24 22 8	-6.76558	14 14 10 10	47.37399	21 21 21 19	-1.01120
14 1 1	2.15469	24 23 1	15.65598	14 14 11 10	14.22759	21 21 21 20	1.67062
15 1 1	-35.91537	24 23 2	-19.56495	14 14 11 11	25.46560	21 21 21 21	13.36894
16 1 1	93.89705	24 23 3	177.29194	14 14 12 10	25.55572	22 17 1 1	-6.97711
17 1 1	7.14862	24 23 4	2.05156	14 14 12 11	20.74590	22 17 2 2	-0.13955
18 1 1	-105.09043	24 23 5	3.24667	14 14 12 12	61.28689	22 17 3 3	0.59420
19 1 1	15.03338	24 23 6	-9.37955	14 14 13 10	32.41999	22 17 4 4	-3.55466
20 1 1	191.52726	24 23 7	28.08815	14 14 13 11	9.14994	22 17 5 5	-0.74584
21 1 1	-3.25728	24 23 8	6.20568	14 14 13 12	26.00748	22 17 6 6	1.04921
22 1 1	9.11906	24 24 1	22.43484	14 14 13 13	42.29466	22 17 7 7	0.08268
23 1 1	47.97150	24 24 2	-113.17749	14 14 14 14	38.42123	22 17 8 8	-3.11731
24 1 1	-0.34941	24 24 3	173.79839	15 14 1 1	-43.28942	22 17 9 9	1.64986
25 1 1	6.63890	24 24 4	-143.67234	15 14 2 2	45.80266	22 17 10 10	-1.69742
26 1 1	51.74096	24 24 5	-45.66686	15 14 3 3	-14.77730	22 17 11 11	1.74830
27 1 1	18.41520	24 24 6	10.11598	15 14 4 4	-2.95424	22 17 12 12	-1.98413
28 1 1	25.05531	24 24 7	-36.59157	15 14 5 5	2.38375	22 17 13 13	5.73528
29 1 1	50.17081	24 24 8	23.93729	15 14 6 6	3.84982	22 17 14 14	-0.85873
30 1 1	133.62801	24 24 9	-15.27022	15 14 7 7	-5.76955	22 17 15 15	1.58339
31 1 1	36.75823	I J K L	F(I,J,K,L)	15 14 8 8	5.47686	22 17 16 16	-2.43633
32 1 1	-24.06997	1 1 1 1	161.35612	15 14 9 9	4.01712	22 17 17 17	-6.74507
33 1 1	2.51606	2 1 1 1	-0.86758	15 14 10 10	-20.91930	22 18 1 1	-3.01631
34 1 1	-87.80793	3 1 1 1	29.53977	15 14 11 11	21.80121	22 18 2 2	-3.37328
35 1 1	100.68977	4 1 1 1	-5.79162	15 14 12 12	26.10654	22 18 3 3	1.62807
36 1 1	-43.43824	5 1 1 1	181.48801	15 14 13 13	7.70274	22 18 4 4	-0.55022
37 1 1	-1.37404	6 1 1 1	29.31218	15 14 14 14	-17.79505	22 18 5 5	0.30275
38 1 1	-3.19672	7 1 1 1	-54.23981	15 15 1 1	-85.39179	22 18 7 7	1.81161
39 1 1	4.59170	8 1 1 1	20.58568	15 15 2 2	-19.13469	22 18 8 8	-1.39996
40 1 1	-19.64891	9 1 1 1	81.18437	15 15 3 3	-62.73311	22 18 9 9	-1.89303
41 1 1	16.47901	10 1 1 1	111.98144	15 15 4 4	31.79303	22 18 10 10	0.45178
42 1 1	-16.73692	11 1 1 1	10.36011	15 15 5 5	14.65002	22 18 11 11	1.90957
43 1 1	-1.25240	12 1 1 1	72.55181	15 15 6 6	-78.38961	22 18 12 12	-3.14151
44 1 1	16.78253	13 1 1 1	-11.33177	15 15 7 7	15.15 4 1	22 18 13 13	2.20300
45 1 1	-50.95811	14 1 1 1	-13.68369	15 15 8 8	-2.30037	22 18 14 14	0.22565
46 1 1	11.84227	15 1 1 1	92.19791	15 15 9 9	-7.03662	22 18 15 15	3.28971
47 1 1	-32.77374	16 1 1 1	-6.97361	15 15 10 10	7.65024	22 18 16 16	-1.53460
48 1 1	24.61206	17 1 1 1	10.29994	15 15 11 11	-2.66908	22 18 17 17	-2.96183
49 1 1	25.80146	18 1 1 1	0.92011	15 15 12 12	-0.52682	22 18 18 18	-0.30659
50 1 1	-16.80937	19 1 1 1	17.45331	15 15 13 13	-2.90125	22 18 19 19	-3.24366
51 1 1	-39.53483	20 1 1 1	-19.26650	15 15 14 14	-0.57741	22 18 20 20	5.45685
52 1 1	-31.60633	21 1 1 1	2.63100	15 15 15 15	1.35745	22 19 1 1	-6.78565
53 1 1	57.30608	22 1 1 1	-0.25276	15 15 16 16	1.57474	22 19 2 2	-9.60745
54 1 1	-6.26722	23 1 1 1	11.96029	15 15 17 17	-0.53739	22 19 3 3	-1.69491
55 1 1	28.94921	24 1 1 1	-16.47470	15 15 18 18	1.44074	22 19 4 4	1.23991
56 1 1	3.39660	25 1 1 1	-3.92962	15 15 19 19	1.96700	22 19 5 5	0.46201
57 1 1	22.57136	26 1 1 1	-0.64844	15 15 20 20	3.70139	22 19 6 6	0.86351
58 1 1	4.01286	27 1 1 1	-6.91919	15 15 21 21	6.74225	22 19 7 7	2.41953
59 1 1		28 1 1 1		15 15 22 22	-1.31160	22 19 8 8	1.38555
60 1 1		29 1 1 1		15 15 23 23	-2.39647	22 19 9 9	0.98817
61 1 1		30 1 1 1		15 15 24 24		22 19 10 10	

I J K	F(I,J,K)	I J K L	F(I,J,,K,L)	I J K L	F(I,J,K,L)	I J K L	F(I,J,K,L)
18 14 12	128.24324	9 7 6 6	-2.54317	19 17 6 6	19.54624	23 23 4 2	-6.06532
18 14 13	167.99222	9 7 7 1	0.77653	19 17 7 7	6.71336	23 23 4 3	5.05261
18 15 10	-86.11417	9 7 7 2	3.40050	19 17 8 8	-18.13781	23 23 4 4	1.05963
18 15 11	-170.43420	9 7 7 3	0.78636	19 17 9 9	3.26701	23 23 5 1	2.05217
18 15 12	-57.72258	9 7 7 4	-2.97593	19 17 10 10	-22.98714	23 23 5 2	-4.27586
18 15 13	5.16200	9 7 7 5	3.75955	19 17 11 11	39.97238	23 23 5 3	1.61172
18 16 10	53.93176	9 7 7 6	2.71264	19 17 12 12	-39.71615	23 23 5 4	-2.48884
18 16 11	31.28737	9 7 7 7	10.33796	19 17 13 13	29.49798	23 23 5 5	7.82042
18 16 12	-68.21644	9 8 1 1	46.53305	19 17 14 14	-1.11090	23 23 6 1	-0.92576
18 16 13	-13.17710	9 8 2 2	12.85780	19 17 15 15	30.93199	23 23 6 2	-3.39377
18 17 1	264.51457	9 8 3 3	33.24473	19 17 16 16	-47.32792	23 23 6 3	4.27087
18 17 2	-4.32609	9 8 4 4	-1.72143	19 17 17 17	35.07040	23 23 6 4	2.04846
18 17 3	-111.99173	9 8 5 5	-0.60970	19 18 1 1	-52.95614	23 23 6 5	8.68688
18 17 4	-5.32632	9 8 6 6	-12.51864	19 18 2 2	80.66402	23 23 6 6	13.39520
18 17 5	-12.03304	9 8 7 7	-5.21232	19 18 3 3	-13.87734	23 23 7 1	0.21570
18 17 6	-2.78040	9 8 8 2	0.59039	19 18 4 4	-9.49076	23 23 7 2	-0.38934
18 17 7	6.06764	9 8 8 3	0.24503	19 18 5 5	-1.26920	23 23 7 3	-2.53032
18 17 8	-5.34169	9 8 8 4	-0.43542	19 18 6 6	17.44795	23 23 7 4	-10.86503
18 17 9	8.42973	9 8 8 5	-10.35017	19 18 7 7	-33.61236	23 23 7 5	7.08876
18 18 1	28.97250	9 8 8 6	1.41974	19 18 8 8	14.51110	23 23 7 6	-0.53164
18 18 2	637.32749	9 8 8 7	2.97991	19 18 9 9	12.12802	23 23 7 7	29.63031
18 18 3	199.94950	9 8 8 8	-20.97055	19 18 10 10	-37.90998	23 23 8 1	0.88537
18 18 4	89.89406	9 9 1 1	-41.82836	19 18 11 11	28.23473	23 23 8 2	1.11851
18 18 5	50.90549	9 9 2 1	-5.04354	19 18 12 12	12.16889	23 23 8 3	1.16188
18 18 6	-9.68455	9 9 2 2	-16.44965	19 18 13 13	4.67028	23 23 8 4	2.93004
18 18 7	-9.22746	9 9 3 1	3.81699	19 18 14 14	-29.64120	23 23 8 5	3.48077
18 18 8	-19.30385	9 9 3 2	12.09921	19 18 15 15	15.60339	23 23 8 6	-1.06664
18 18 9	-11.07694	9 9 3 3	-33.81499	19 18 16 16	19.78867	23 23 8 7	-7.78536
19 14 10	38.91265	9 9 4 1	0.13339	19 18 17 17	-51.08031	23 23 8 8	25.44966
19 14 11	125.50182	9 9 4 2	-4.49934	19 18 18 18	-27.59740	23 23 9 1	-0.73686
19 14 12	101.03799	9 9 4 3	5.02484	19 18 19 19	77.91699	23 23 9 2	0.29553
19 14 13	-17.08954	9 9 4 4	-5.55423	19 19 1 1	111.35247	23 23 9 3	-0.20122
19 15 10	-131.62565	9 9 5 1	1.21041	19 19 2 1	10.38438	23 23 9 4	-3.49179
19 15 11	157.49796	9 9 5 2	-2.34085	19 19 2 2	73.17202	23 23 9 5	0.44481
19 15 12	-80.84608	9 9 5 3	3.89524	19 19 3 1	-11.46664	23 23 9 6	6.12636
19 15 13	-191.42873	9 9 5 4	6.08694	19 19 3 2	-13.02898	23 23 9 7	12.27550
19 16 10	-71.99058	9 9 5 5	2.15584	19 19 3 3	91.76915	23 23 9 8	-24.21541
19 16 11	13.18317	9 9 6 1	1.59309	19 19 4 1	-0.09834	23 23 9 9	28.33687
19 16 12	234.20550	9 9 6 2	-1.04736	19 19 4 2	12.07657	23 23 10 10	12.48813
19 16 13	41.40566	9 9 6 3	3.56203	19 19 4 3	-16.30755	23 23 11 10	1.41708
19 17 1	-537.94798	9 9 6 4	4.05278	19 19 4 4	-2.53473	23 23 11 11	13.08131
19 17 2	-91.85513	9 9 6 5	8.59163	19 19 5 1	-1.56069	23 23 12 10	3.35362
19 17 3	-13.81708	9 9 6 6	15.75550	19 19 5 2	10.20100	23 23 12 11	4.77962
19 17 4	4.16527	9 9 7 1	-1.25524	19 19 5 3	-6.43932	23 23 12 12	30.03597
19 17 5	-0.34735	9 9 7 2	2.46135	19 19 5 4	1.21854	23 23 13 10	8.78127
19 17 6	5.14362	9 9 7 4	-3.87756	19 19 5 5	-14.38160	23 23 13 11	-3.86671
19 17 7	-8.09591	9 9 7 5	1.02169	19 19 6 1	0.14467	23 23 13 12	11.62049
19 17 8	3.65834	9 9 7 6	-5.57991	19 19 6 2	5.22497	23 23 13 13	6.11628
19 17 9	-11.42047	9 9 7 7	8.02174	19 19 6 3	-12.00375	23 23 14 14	8.97956
19 18 1	-105.11546	9 9 8 2	0.31535	19 19 6 4	-6.65285	23 23 15 14	-1.51953
19 18 2	207.67050	9 9 8 3	0.43569	19 19 6 5	-14.48779	23 23 15 15	15.00961
19 18 3	364.38471	9 9 8 4	-2.41264	19 19 6 6	-33.19292	23 23 16 14	3.56519
19 18 4	-33.47585	9 9 8 5	7.27955	19 19 7 1	1.33097	23 23 16 15	1.53394
19 18 5	5.90356	9 9 8 6	-4.64829	19 19 7 2	-0.28225	23 23 16 16	9.30894
19 18 6	-21.89795	9 9 8 7	-0.83597	19 19 7 3	3.21052	23 23 17 17	-47.44588
19 18 7	-7.07585	9 9 8 8	21.36156	19 19 7 4	11.79373	23 23 18 17	2.14607
19 18 8	1.15551	9 9 9 1	0.96298	19 19 7 5	-3.68986	23 23 18 18	-61.12806
19 18 9	-0.92356	9 9 9 2	0.82109	19 19 7 6	6.37605	23 23 19 17	-1.24227
19 19 1	-0.25231	9 9 9 3	-1.06636	19 19 7 7	-23.63885	23 23 19 18	-12.08192
19 19 2	364.70637	9 9 9 4	1.41149	19 19 8 1	-6.26091	23 23 19 19	-48.07357
19 19 3	-291.41143	9 9 9 5	-0.60687	19 19 8 2	-1.85645	23 23 20 17	1.98244
19 19 4	95.65694	9 9 9 6	12.32500	19 19 8 3	0.55756	23 23 20 18	-9.20101
19 19 5	51.51235	9 9 9 7	0.47249	19 19 8 4	-1.71181	23 23 20 19	4.55400
19 19 6	16.43348	9 9 9 8	-23.66549	19 19 8 5	-10.21159	23 23 20 20	0.60204
19 19 7	3.97853	9 9 9 9	34.44953	19 19 8 6	8.27085	23 23 21 17	1.49742
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23 17 9	17.33803	13 11 7 7	0.86323	21 18 16 16	-1.56078	24 24 6 4	12.97483
23 18 1	7.91846	13 11 8 8	-6.49915	21 18 17 17	0.50095	24 24 6 5	14.40818
23 18 2	1.17269	13 11 9 9	-9.53775	21 18 18 17	-0.63108	24 24 6 6	30.30333
23 18 3	-2.30118	13 11 10 10	13.02315	21 19 1 1	3.81510	24 24 7 1	-1.29278
23 18 4	33.03805	13 11 11 10	24.52388	21 19 2 2	-2.19938	24 24 7 2	0.74295
23 18 5	-49.38977	13 11 11 11	-71.15824	21 19 3 3	-7.70333	24 24 7 3	-2.78883
23 18 6	-43.37562	13 12 1 1	-11.91661	21 19 4 4	4.18202	24 24 7 4	-11.35098
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23 18 9	-96.59721	13 12 4 4	14.44617	21 19 8 8	3.43888	24 24 7 7	12.52887
23 19 1	-8.10708	13 12 5 5	-2.30480	21 19 9 9	3.79554	24 24 8 1	-3.31204
23 19 2	-2.09039	13 12 6 6	3.33583	21 19 10 10	0.60362	24 24 8 2	-1.34173
23 19 3	3.71012	13 12 7 7	6.54563	21 19 11 11	-3.13302	24 24 8 3	0.88446
23 19 4	26.81928	13 12 8 8	4.49990	21 19 12 12	5.91750	24 24 8 4	6.84485
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I J K	Fl(I,J,K)	I J K L	Fl(I,J,,K,L)	I J K L	Fl(I,J,K,L)	I J K L	Fl(I,J,K,L)
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8 8 2	-5.87605	6 4 4 4	-17.76752	14 14 8 5	-0.45308	20 16 1 1	-0.12102
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16 13 11	-197.95556	8 6 6 1	-0.37514	16 16 13 13	-256.44483	20 20 16 15	-5.80807
16 14 9	78.13763	8 6 6 2	0.33751	16 16 14 12	41.53057	20 20 16 16	-2.06628
16 14 10	53.90201	8 6 6 3	-2.70918	16 16 14 13	40.81964	20 20 17 15	-1.77062
16 14 11	37.40848	8 6 6 4	1.26892	16 16 14 14	-7.90518	20 20 17 16	1.08379

I J K	FI(I,J,K)	I J K L	FI(I,J,K,L)	I J K L	FI(I,J,K,L)	I J K L	FI(I,J,K,L)
16 15 1	-173.48513	8 6 6 5	-7.30539	16 16 15 15	30.91569	20 20 17 17	-10.20131
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16 15 3	0.30937	8 7 2 2	10.90620	16 16 16 16	523.74555	20 20 18 16	-1.20783
16 15 4	3.04173	8 7 3 3	-1.71264	17 15 1 1	-19.23827	20 20 18 17	1.73981
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16 15 6	1.19269	8 7 5 5	-3.20719	17 15 3 3	2.36535	20 20 19 15	-3.18549
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16 16 5	-8.87307	8 7 7 6	3.13356	17 15 10 10	14.54512	20 20 20 18	-1.73730
16 16 6	-25.98638	8 7 7 7	9.41675	17 15 11 11	-1.28918	20 20 20 19	-4.92504
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17 15 2	3.63874	8 8 5 3	1.29191	17 16 9 9	0.15420	21 15 13 13	0.61257
17 15 3	36.16176	8 8 5 4	0.27785	17 16 10 10	2.14804	21 15 15 15	-1.13128
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17 15 8	-16.48582	8 8 6 4	-1.30691	17 16 15 15	-2.65725	21 16 5 5	1.21949
17 16 1	-1.77772	8 8 6 6	1.70956	17 16 16 15	-3.47902	21 16 6 6	3.48674
17 16 2	28.11226	8 8 7 1	-1.32158	17 16 16 16	13.03092	21 16 7 7	-0.21071
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17 16 7	-56.48753	8 8 7 6	0.71842	17 17 3 2	-5.94673	21 16 13 13	0.39015
17 16 8	23.04278	8 8 7 7	4.52125	17 17 3 3	31.00221	21 16 15 15	-0.23464
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17 17 6	-70.84292	8 8 8 6	0.77089	17 17 5 3	-2.82015	21 17 5 5	-11.10681
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17 17 8	-4.86385	8 8 8 8	-2.07821	17 17 5 5	21.48474	21 17 7 7	-7.22326
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18 12 10	10.71248	9 9 2 1	66.45195	17 17 6 2	-1.55609	21 17 9 9	-8.29789
18 12 11	19.47043	9 9 2 2	-319.41855	17 17 6 3	-21.48476	21 17 10 10	-5.20810
18 13 9	9.60640	9 9 3 1	0.10756	17 17 6 4	-2.13610	21 17 11 11	-1.83704
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18 14 9	13.17393	9 9 4 1	-1.09628	17 17 7 1	0.46449	21 17 14 14	0.88141
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18 14 11	19.45612	9 9 4 3	6.54226	17 17 7 3	12.17920	21 17 16 16	32.73493
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18 15 2	2.01734	9 9 5 1	0.81504	17 17 7 5	4.65507	21 17 17 16	1.12298
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18 15 4	-177.72719	9 9 5 3	22.32948	17 17 7 7	-2.50427	21 18 1 1	19.90336
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18 15 6	125.78802	9 9 5 5	28.61996	17 17 8 2	-0.54536	21 18 3 3	10.47457
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18 16 3	138.34259	9 9 6 6	10.43765	17 17 8 7	1.18081	21 18 8 8	-0.30365
18 16 4	25.40871	9 9 7 1	-0.86116	17 17 8 8	-1.13883	21 18 9 9	12.59228
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18 16 6	-81.42864	9 9 7 3	14.78543	17 17 10 9	-0.42352	21 18 11 11	2.24159
18 16 7	84.67077	9 9 7 4	7.22189	17 17 10 10	5.57677	21 18 12 12	4.77908
18 16 8	-45.11465	9 9 7 5	13.80425	17 17 11 9	12.42904	21 18 13 13	4.41484
18 17 1	41.56590	9 9 7 6	-9.93228	17 17 11 10	4.10200	21 18 14 14	1.89139
18 17 2	124.72557	9 9 7 7	7.08736	17 17 11 11	-17.49808	21 18 15 15	22.19141
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I J K	Fl(I,J,K)	I J K L	Fl(I,J,K,L)	I J K L	Fl(I,J,K,L)	I J K L	Fl(I,J,K,L)
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19 12 10	21.25970	10 9 6 6	-2.86349	18 15 3 3	1.75821	21 19 9 9	-10.61359
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19 13 9	6.89393	10 9 8 8	-0.24285	18 15 5 5	0.37156	21 19 11 11	-2.36011
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19 14 9	-5.62499	10 10 2 1	-107.40853	18 15 8 8	1.37846	21 19 14 14	-0.93033
19 14 10	-2.04643	10 10 2 2	-70.65502	18 15 9 9	0.30130	21 19 15 15	28.03475
19 14 11	-20.90538	10 10 3 1	2.29176	18 15 10 10	2.67310	21 19 16 16	36.60097
19 15 1	-10.56446	10 10 3 2	-1.02254	18 15 11 11	-0.13254	21 19 17 17	-5.91616
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20 18 5	-30.12367	11 11 7 5	3.73406	18 18 10 10	43.54037	21 21 15 15	-6.33004
20 18 6	6.44732	11 11 7 6	-3.32488	18 18 11 9	11.52472	21 21 16 15	2.12810

I	J	K	FI(I,J,K)	I	J	K	L	FI(I,J,K,L)	I	J	K	L	FI(I,J,K,L)	I	J	K	L	FI(I,J,K,L)
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20	18	8	-17.56546	11	11	8	1	-0.44621	18	18	11	11	0.80961	21	21	17	15	-0.10804
20	19	1	-94.72586	11	11	8	4	-0.65126	18	18	12	12	29.12506	21	21	17	16	-1.48854
20	19	2	-36.44523	11	11	8	5	-2.20346	18	18	13	12	1.18335	21	21	17	17	2.22909
20	19	3	5.27688	11	11	8	6	1.95536	18	18	13	13	44.81029	21	21	18	15	-0.85060
20	19	4	11.17237	11	11	8	7	-0.62830	18	18	14	12	-8.88863	21	21	18	16	1.34041
20	19	5	-8.12232	11	11	9	9	69.86832	18	18	14	13	1.08360	21	21	18	17	-1.32616
20	19	6	-34.97243	11	11	10	9	10.03826	18	18	14	14	-3.94883	21	21	18	18	8.58838
20	19	7	24.26298	11	11	10	10	26.48361	18	18	15	15	-118.09641	21	21	19	15	-0.15476
20	19	8	-4.12535	11	11	11	9	14.09307	18	18	16	15	1.32815	21	21	19	16	-0.88471
20	20	1	35.85982	11	11	11	10	16.05960	18	18	16	16	-129.91401	21	21	19	17	2.78310
20	20	2	13.18999	11	11	11	11	24.50286	18	18	17	15	3.97203	21	21	19	18	-2.53466
20	20	3	-17.00584	12	12	1	1	-204.74608	18	18	17	16	0.27275	21	21	19	19	5.80862
20	20	4	13.43689	12	12	2	1	1.29998	18	18	17	17	16.68498	21	21	20	15	0.15732
20	20	5	19.14540	12	12	2	2	-218.48656	18	18	18	15	2.53710	21	21	20	16	0.45301
20	20	6	-9.51301	12	12	3	1	-1.25396	18	18	18	16	5.79176	21	21	20	17	2.54876
20	20	7	-49.77687	12	12	3	2	-0.19284	18	18	18	17	-12.52116	21	21	20	18	3.00449
20	20	8	-28.37975	12	12	3	3	10.79807	18	18	18	18	52.39754	21	21	20	19	-2.20026
21	12	9	6.88598	12	12	4	1	-4.42589	19	15	1	1	2.56154	21	21	20	20	5.12117
21	12	10	-12.95504	12	12	4	2	0.45389	19	15	2	2	0.25647	21	21	21	15	0.75661
21	12	11	-2.59617	12	12	4	3	2.90365	19	15	3	3	0.49289	21	21	21	16	0.51553
21	13	9	0.62671	12	12	4	4	14.29157	19	15	4	4	4.05746	21	21	21	17	-4.47358
21	13	10	-2.73868	12	12	5	1	3.39634	19	15	5	5	-2.83817	21	21	21	18	-4.78494
21	13	11	-3.94363	12	12	5	2	-2.58727	19	15	6	6	-2.37205	21	21	21	19	-2.22505
21	14	9	0.90056	12	12	5	3	16.30930	19	15	7	7	-1.61578	21	21	21	20	-9.32639
21	14	11	5.60459	12	12	5	4	-10.41233	19	15	8	8	1.90517	21	21	21	21	16.74697
21	15	1	4.41596	12	12	5	5	33.54148	19	15	9	9	1.32901					
21	15	2	1.37905	12	12	6	1	-1.68352	19	15	10	10	-3.11176					

Table S43: The quartic potential energy surface of Thiophene-d4. The calculation was done by using B3LYP/6-311++G(2d,2p) method. The force constants (F_I) are in cm⁻¹ units.

I J	F _I (I,J)	I J K	F _I (I,J,K)	I J K L	F _I (I,J,K,L)	I J K L	F _I (I,J,K,L)
1 1	2417.81227	21 15 6	66.54527	12 12 6 6	12.20272	19 15 14 14	0.64627
2 2	2376.61514	21 15 7	-5.65723	12 12 7 1	-1.68121	19 15 15 15	-6.27601
3 3	1403.63729	21 15 8	18.31646	12 12 7 2	-2.05403	19 16 1 1	-4.78870
4 4	1265.19821	21 16 1	-3.56067	12 12 7 3	3.82223	19 16 2 2	-3.93378
5 5	901.67754	21 16 2	17.38951	12 12 7 4	6.76316	19 16 3 3	-3.36269
6 6	798.70722	21 16 3	32.28029	12 12 7 5	-5.75618	19 16 4 4	-4.20965
7 7	735.08106	21 16 4	34.54839	12 12 7 6	-3.84324	19 16 5 5	0.86791
8 8	594.13073	21 16 5	-32.49507	12 12 7 7	9.69153	19 16 6 6	-0.65249
9 9	767.90298	21 16 6	-59.21231	12 12 8 1	-1.56279	19 16 7 7	-0.21306
10 10	533.76588	21 16 7	82.92034	12 12 8 2	0.52968	19 16 8 8	0.33227
11 11	495.37316	21 16 8	-16.38731	12 12 8 3	-2.10549	19 16 9 9	0.41385
12 12	702.50967	21 17 1	-31.78849	12 12 8 4	1.13341	19 16 10 10	0.84321
13 13	539.52261	21 17 2	24.51461	12 12 8 5	-3.23716	19 16 11 11	2.37947
14 14	421.91169	21 17 3	39.75310	12 12 8 6	5.23798	19 16 12 12	2.59632
15 15	2409.02605	21 17 4	-16.87750	12 12 8 7	-0.28732	19 16 13 13	2.59211
16 16	2361.75934	21 17 5	21.56355	12 12 8 8	0.56810	19 16 14 14	0.92006
17 17	1487.12065	21 17 6	-3.36828	12 12 9 9	39.11047	19 16 15 15	-5.15984
18 18	1043.48636	21 17 7	22.57831	12 12 10 9	1.40315	19 16 16 15	2.81776
19 19	860.79530	21 17 8	3.68839	12 12 10 10	97.22788	19 16 16 16	-7.63965
20 20	764.04221	21 18 1	5.67861	12 12 11 9	-51.02424	19 17 1 1	11.23702
21 21	711.63857	21 18 2	78.77875	12 12 11 10	13.33620	19 17 2 2	20.78536
		21 18 3	-7.74651	12 12 11 11	43.45665	19 17 3 3	10.21229
I J K	F _I (I,J,K)	21 18 4	38.53803	12 12 12 12	37.88931	19 17 4 4	7.50378
		21 18 5	-44.55601	13 12 1 1	62.27658	19 17 5 5	-0.99479
1 1 1	-669.34054	21 18 6	-9.02336	13 12 2 2	-67.90301	19 17 6 6	-5.95213
2 1 1	-155.75720	21 18 7	-33.54570	13 12 3 3	6.59002	19 17 7 7	-7.10421
2 2 1	-476.29663	21 18 8	-35.85248	13 12 4 4	-1.83455	19 17 8 8	-1.48268
2 2 2	504.13705	21 19 1	39.09473	13 12 5 5	-5.94295	19 17 9 9	-4.36915
3 1 1	72.88802	21 19 2	-48.83302	13 12 6 6	3.51238	19 17 10 10	-2.80050
3 2 1	23.59625	21 19 3	-1.33821	13 12 7 7	9.83105	19 17 11 11	-4.53841
3 2 2	10.09948	21 19 4	8.52854	13 12 8 8	-1.09880	19 17 12 12	-4.90960
3 3 1	87.68736	21 19 5	2.67327	13 12 9 9	65.67555	19 17 13 13	-4.35262
3 3 2	-81.08136	21 19 6	3.33784	13 12 10 10	-118.30726	19 17 14 14	-4.15208
3 3 3	129.37739	21 19 7	-4.85787	13 12 11 11	56.78515	19 17 15 15	9.42735
4 1 1	-51.16347	21 19 8	-5.97025	13 12 12 12	17.59781	19 17 16 16	22.03042
4 2 1	28.84680	21 20 1	-55.06461	13 13 1 1	-137.42420	19 17 17 15	1.19320
4 2 2	-80.83329	21 20 2	-5.12626	13 13 2 1	1.63164	19 17 17 16	-0.69811
4 3 1	-21.66597	21 20 3	-5.34768	13 13 2 2	-144.21977	19 17 17 17	16.56020
4 3 2	-57.76723	21 20 4	18.04336	13 13 3 1	10.55009	19 18 1 1	-3.15716
4 3 3	-219.54829	21 20 5	-32.60263	13 13 3 2	2.88407	19 18 2 2	33.50981
4 4 1	66.38089	21 20 6	-11.62267	13 13 3 3	2.53836	19 18 3 3	-9.31979
4 4 2	-0.89254	21 20 7	-26.67959	13 13 4 1	-10.52932	19 18 4 4	0.59427
4 4 3	-45.87044	21 20 8	-28.77562	13 13 4 2	10.39224	19 18 5 5	2.49217
4 4 4	-91.19211	21 21 1	46.29396	13 13 4 3	1.19292	19 18 6 6	-6.71843
5 1 1	-46.64606	21 21 2	-37.22644	13 13 4 4	1.74769	19 18 7 7	-8.13069
5 2 1	0.41604	21 21 3	-2.65052	13 13 5 1	-8.74272	19 18 8 8	1.45138
5 2 2	-48.39903	21 21 4	41.39300	13 13 5 2	2.62377	19 18 9 9	-5.97597
5 3 1	19.66556	21 21 5	-51.29302	13 13 5 3	1.36790	19 18 10 10	2.96575
5 3 2	8.08530	21 21 6	6.73424	13 13 5 4	-7.36761	19 18 11 11	-4.28610
5 3 3	-112.42026	21 21 7	-56.84776	13 13 5 5	7.67594	19 18 12 12	-4.14486
5 4 1	-45.45761	21 21 8	-60.89026	13 13 6 1	-0.44900	19 18 13 13	-6.54614
5 4 2	-41.05191			13 13 6 2	-0.81500	19 18 15 15	-9.40667
5 4 3	-53.19996	I J K L	F _I (I,J,K,L)	13 13 6 3	-10.17236	19 18 16 16	39.74828
5 4 4	-100.43247			13 13 6 4	2.56779	19 18 17 17	-7.48243
5 5 1	80.15575	1 1 1 1	186.62221	13 13 6 5	-6.95482	19 18 18 15	-0.42394
5 5 2	20.48247	2 1 1 1	67.64311	13 13 6 6	23.36326	19 18 18 16	0.98148
5 5 3	-54.86432	2 2 1 1	96.89946	13 13 7 1	-1.25021	19 18 18 17	-5.56689
5 5 4	-30.65724	2 2 2 1	-66.74040	13 13 7 2	-1.34951	19 18 18 18	-4.04946
5 5 5	-95.28668	2 2 2 2	192.02892	13 13 7 3	6.61694	19 19 1 1	-13.50880
6 1 1	-5.37258	3 1 1 1	-17.96587	13 13 7 4	10.25289	19 19 2 1	14.26521
6 2 1	-3.52631	3 2 1 1	-8.72897	13 13 7 5	-9.76870	19 19 2 2	-33.97105
6 2 2	3.86614	3 2 2 1	-5.88263	13 13 7 6	-7.07693	19 19 3 2	-3.35623
6 3 1	-34.83960	3 2 2 2	-1.73763	13 13 7 7	17.28799	19 19 3 3	-4.40980
6 3 2	37.30514	3 3 1 1	-3.02750	13 13 8 1	-0.53082	19 19 4 1	-1.13020
6 3 3	32.64184	3 3 2 1	4.54344	13 13 8 2	1.35263	19 19 4 2	2.01326
6 4 1	35.62635	3 3 2 2	-15.84771	13 13 8 3	-4.43260	19 19 4 3	-0.54513
6 4 2	57.18942	3 3 3 1	8.87718	13 13 8 4	2.28064	19 19 4 4	1.35584
6 4 3	-41.59551	3 3 3 2	63.06879	13 13 8 5	-4.73290	19 19 5 1	-0.40540
6 4 4	-2.95420	4 1 1 1	10.73656	13 13 8 6	10.44358	19 19 5 2	0.25139
6 5 1	-62.26218	4 2 1 1	-2.33856	13 13 8 7	-0.52406	19 19 5 3	-2.16122
6 5 2	-61.09874	4 2 2 1	13.11136	13 13 8 8	2.95872	19 19 5 4	-1.14973
6 5 3	-19.51901	4 2 2 2	-22.84167	13 13 9 9	86.71148	19 19 5 5	1.47135
6 5 4	-16.88361	4 3 1 1	1.38692	13 13 10 9	7.99159	19 19 6 1	1.04151
6 5 5	-15.57758	4 3 2 2	-7.59995	13 13 10 10	168.14671	19 19 6 2	-1.03047
6 6 1	131.30810	4 3 3 1	-12.37452	13 13 11 9	-77.72055	19 19 6 3	-4.69006
6 6 2	-48.53656	4 3 3 2	6.22305	13 13 11 10	24.61474	19 19 6 4	-2.98990
6 6 3	-2.95619	4 3 3 3	-6.21584	13 13 11 11	68.23253	19 19 6 5	0.63662
6 6 4	-8.40753	4 4 1 1	-22.93521	13 13 12 12	118.39626	19 19 6 6	12.11987
6 6 5	-3.96452	4 4 2 1	-8.73733	13 13 13 12	17.23205	19 19 7 1	0.19238
6 6 6	-3.47079	4 4 2 2	-11.68767	13 13 13 13	188.75840	19 19 7 2	0.86638
7 1 1	-14.82034	4 4 3 1	1.14670	14 12 1 1	52.41178	19 19 7 3	6.89340
7 2 1	-9.99768	4 4 3 2	10.32927	14 12 2 2	30.38450	19 19 7 4	2.58771
7 2 2	-4.10996	4 4 3 3	29.25007	14 12 3 3	-9.95660	19 19 7 5	-3.23344
7 3 1	23.70573	4 4 4 1	-4.35070	14 12 4 4	-4.07478	19 19 7 6	-8.70185
7 3 2	-49.47572	4 4 4 2	3.11535	14 12 5 5	-5.01810	19 19 7 7	10.08232

I J K	F(I,J,K)	I J K L	F(I,J,,K,L)	I J K L	F(I,J,K,L)	I J K L	F(I,J,K,L)
16 15 1	-123.78201	8 7 1 1	-10.42770	16 16 14 13	13.27941	20 20 18 16	0.47210
16 15 2	-373.57249	8 7 2 2	9.10785	16 16 14 14	-9.62468	20 20 18 17	-8.43801
16 15 3	6.94111	8 7 3 3	0.13243	16 16 15 15	59.07038	20 20 18 18	20.27765
16 15 4	19.16969	8 7 4 4	3.31623	16 16 16 15	-71.14239	20 20 19 15	1.02945
16 15 5	-1.70127	8 7 5 5	6.56618	16 16 16 16	235.07684	20 20 19 16	0.68187
16 15 6	-1.91324	8 7 6 6	-1.87905	17 15 1 1	-25.07695	20 20 19 17	-3.09639
16 15 7	-9.67584	8 7 7 1	-1.20889	17 15 2 2	-14.20475	20 20 19 18	5.28118
16 15 8	3.71678	8 7 7 2	-0.14065	17 15 3 3	12.98113	20 20 19 19	3.21905
16 16 1	-443.45662	8 7 7 3	-3.20654	17 15 4 4	4.02591	20 20 20 15	-2.44696
16 16 2	631.14322	8 7 7 4	-1.93168	17 15 5 5	1.78623	20 20 20 16	-1.46192
16 16 3	22.47610	8 7 7 5	2.44107	17 15 6 6	7.24887	20 20 20 17	12.05678
16 16 4	-77.02481	8 7 7 6	8.09174	17 15 7 7	2.69713	20 20 20 18	-26.11787
16 16 5	-41.12404	8 7 7 7	-1.54565	17 15 8 8	1.00083	20 20 20 19	-10.57859
16 16 6	3.34692	8 8 1 1	-11.90072	17 15 9 9	0.65731	20 20 20 20	39.85177
16 16 7	-0.49055	8 8 2 1	-3.88885	17 15 10 10	24.46313	21 15 1 1	-1.38365
16 16 8	-8.81632	8 8 2 2	-6.71082	17 15 11 11	-0.14228	21 15 2 2	-2.46812
17 12 9	19.90160	8 8 3 1	0.62478	17 15 12 12	7.64789	21 15 3 3	-0.17218
17 12 10	21.19019	8 8 3 2	0.36986	17 15 13 13	17.61928	21 15 4 4	-0.36556
17 12 11	19.71643	8 8 3 3	0.16746	17 15 14 14	1.64633	21 15 5 5	1.61876
17 13 9	-5.83754	8 8 4 1	-0.53910	17 15 15 15	-27.07974	21 15 6 6	0.15471
17 13 10	-31.80687	8 8 4 2	0.20704	17 16 1 1	-2.46899	21 15 7 7	-0.30501
17 13 11	-31.76409	8 8 4 3	0.42711	17 16 2 2	18.47233	21 15 8 8	1.10960
17 14 9	30.41632	8 8 4 4	0.88448	17 16 3 3	-6.95117	21 15 9 9	0.50271
17 14 10	-16.27405	8 8 5 1	-0.86252	17 16 4 4	5.69564	21 15 10 10	1.63798
17 14 11	33.99005	8 8 5 4	-2.48888	17 16 5 5	0.82478	21 15 11 11	0.48450
17 15 1	104.55138	8 8 5 5	5.55054	17 16 6 6	-1.97983	21 15 12 12	-0.13704
17 15 2	8.98071	8 8 6 1	-0.70584	17 16 7 7	-2.49685	21 15 13 13	1.88587
17 15 3	77.28951	8 8 6 2	-0.32677	17 16 8 8	-5.30442	21 15 14 14	-1.31023
17 15 4	-48.11850	8 8 6 3	-0.95295	17 16 9 9	7.65028	21 16 1 1	0.26113
17 15 5	27.50075	8 8 6 4	0.29999	17 16 10 10	-7.86266	21 16 2 2	7.09287
17 15 6	-37.17793	8 8 6 5	-2.23320	17 16 11 11	-2.67343	21 16 3 3	1.32817
17 15 7	7.50985	8 8 6 6	4.60359	17 16 12 12	-6.96550	21 16 4 4	-1.16589
17 15 8	-18.35795	8 8 7 1	-1.10688	17 16 13 13	3.24655	21 16 5 5	2.75088
17 16 1	-16.15651	8 8 7 2	-0.75526	17 16 14 14	-5.94572	21 16 6 6	-0.52233
17 16 2	77.34598	8 8 7 3	0.87510	17 16 15 15	-12.94687	21 16 7 7	-0.26499
17 16 3	-60.85217	8 8 7 4	0.65733	17 16 16 16	24.26676	21 16 8 8	0.36037
17 16 4	-38.01000	8 8 7 5	3.80201	17 17 1 1	-3.51962	21 16 9 9	-1.59598
17 16 5	23.36663	8 8 8 1	-1.51246	17 17 2 2	1.40886	21 16 10 10	0.50138
17 16 6	27.71440	8 8 8 2	-0.39578	17 17 3 3	44.17374	21 16 11 11	-1.79699
17 16 7	-44.47878	8 8 8 3	-1.72511	17 17 4 4	-8.16082	21 16 12 12	-1.94493
17 16 8	5.68652	8 8 8 4	2.45621	17 17 5 5	16.31416	21 16 13 13	-1.79493
17 17 1	78.27420	8 8 8 5	-0.56348	17 17 6 6	-6.72940	21 16 14 14	-1.22264
17 17 2	-18.81532	8 8 8 6	2.75323	17 17 7 7	44.17374	21 16 15 15	-0.98580
17 17 3	253.08159	8 8 8 7	1.35716	17 17 8 8	-8.16082	21 16 16 16	4.80942
17 17 4	-119.04545	8 8 8 8	-0.55027	17 17 9 9	-5.31809	21 17 1 1	10.87544
17 17 5	-55.41403	9 9 1 1	-39.00209	17 17 10 10	-28.67560	21 17 2 2	18.81372
17 17 6	52.75865	9 9 2 1	42.44185	17 17 11 11	1.62794	21 17 3 3	1.24774
17 17 7	16.60144	9 9 2 2	-99.11973	17 17 12 12	0.70264	21 17 4 4	-4.54778
17 17 8	5.19017	9 9 3 1	0.57004	17 17 13 13	2.97896	21 17 5 5	-5.80241
18 12 9	-4.34478	9 9 3 2	-3.40013	17 17 14 14	-9.29383	21 17 6 6	-6.08058
18 12 10	-12.51980	9 9 3 3	-10.32706	17 17 15 15	2.45319	21 17 7 7	-8.91963
18 12 11	-11.80389	9 9 4 1	-2.09400	17 17 16 16	0.81375	21 17 8 8	-0.49112
18 13 9	9.05846	9 9 4 2	4.64653	17 17 17 17	-3.24476	21 17 9 9	-3.22971
18 13 10	3.94266	9 9 4 3	-0.78070	17 17 18 18	1.75901	21 17 10 10	-3.23241
18 13 11	12.15639	9 9 4 4	-10.73829	17 17 19 19	8.18698	21 17 11 11	-3.87253
18 14 9	11.72550	9 9 5 1	-0.64180	17 17 20 20	-4.06248	21 17 12 12	-3.64290
18 14 10	-8.22806	9 9 5 2	1.50789	17 17 21 21	-2.02466	21 17 13 13	-6.95478
18 14 11	-5.31603	9 9 5 3	-3.19763	17 17 22 22	3.39466	21 17 14 14	9.56811
18 15 1	9.06500	9 9 5 4	-6.50551	17 17 23 23	0.75773	21 17 15 15	20.87115
18 15 2	4.98066	9 9 5 5	-2.90354	17 17 24 24	-2.75696	21 17 16 16	-1.07453
18 15 3	-13.66812	9 9 6 1	-0.52693	17 17 25 25	7.67960	21 17 17 17	2.09516
18 15 4	67.51472	9 9 6 2	-1.13553	17 17 26 26	6.06835	21 17 18 18	5.48520
18 15 5	-77.62339	9 9 6 3	-7.67239	17 17 27 27	-2.36257	21 18 1 1	-5.72810
18 15 6	49.56242	9 9 6 4	-2.74953	17 17 28 28	-1.88661	21 18 2 2	28.89919
18 15 7	80.43442	9 9 6 5	0.93371	17 17 29 29	2.55780	21 18 3 3	-4.05464
18 15 8	22.76935	9 9 6 6	8.78030	17 17 30 30	-2.46003	21 18 4 4	2.92308
18 16 1	5.03718	9 9 7 1	-1.05325	17 17 31 31	-0.85471	21 18 5 5	8.38526
18 16 2	1.59379	9 9 7 2	0.78961	17 17 32 32	-0.31486	21 18 6 6	-5.64748
18 16 3	-63.91247	9 9 7 3	6.43444	17 17 33 33	-2.45016	21 18 7 7	-4.57756
18 16 4	-3.55253	9 9 7 4	5.50800	17 17 34 34	2.53785	21 18 8 8	2.93774
18 16 5	-11.98643	9 9 7 5	-1.81193	17 17 35 35	2.29889	21 18 9 9	-6.54037
18 16 6	108.80789	9 9 7 6	-8.67446	17 17 36 36	-1.03847	21 18 10 10	6.04767
18 16 7	-70.96053	9 9 7 7	9.59705	17 17 37 37	-13.67113	21 18 11 11	-5.12040
18 16 8	37.79497	9 9 8 1	-0.99143	17 17 38 38	0.51293	21 18 12 12	-3.32073
18 17 1	-20.22029	9 9 8 2	0.61664	17 17 39 39	0.39445	21 18 13 13	-5.00962
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I	J	K	FI(I,J,K)	I	J	K	L	FI(I,J,,K,L)	I	J	K	L	FI(I,J,K,L)	I	J	K	L	FI(I,J,K,L)
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20	19	3	-13.00132	11	11	9	9	60.33081	18	18	13	12	0.30041	21	21	16	16	-30.53351
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20	19	7	-1.21965	11	11	11	10	16.51133	18	18	14	14	-1.30835	21	21	18	15	1.26360
20	19	8	-10.53352	11	11	11	11	48.29941	18	18	15	15	-47.59228	21	21	18	16	0.38010
20	20	1	144.84015	12	12	1	1	-96.19517	18	18	16	15	2.48712	21	21	18	18	13.27628
20	20	2	69.31395	12	12	2	1	-1.52903	18	18	16	16	-53.69597	21	21	19	15	0.12816
20	20	3	-9.81865	12	12	2	2	-97.60171	18	18	17	15	2.49631	21	21	19	16	-0.24594
20	20	4	10.53895	12	12	3	1	2.88717	18	18	17	16	-0.23845	21	21	19	17	-3.60229
20	20	5	-10.03306	12	12	3	2	2.31474	18	18	17	17	-4.63266	21	21	19	18	-4.57545
20	20	6	-14.69580	12	12	3	3	-4.50578	18	18	18	15	1.13093	21	21	19	19	4.76100
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20	20	8	-11.48878	12	12	4	2	4.07665	18	18	18	17	2.96412	21	21	20	16	-0.16932
21	12	10	-10.55013	12	12	4	3	2.43853	18	18	18	18	13.93135	21	21	20	17	-0.40006
21	13	9	4.47887	12	12	4	4	-2.54572	19	15	1	1	-5.21607	21	21	20	18	3.46877
21	13	10	-10.74282	12	12	5	1	-3.99058	19	15	2	2	0.11794	21	21	20	19	-3.33061
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21	14	9	-0.74842	12	12	5	3	2.29861	19	15	4	4	2.88920	21	21	21	15	1.26945
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