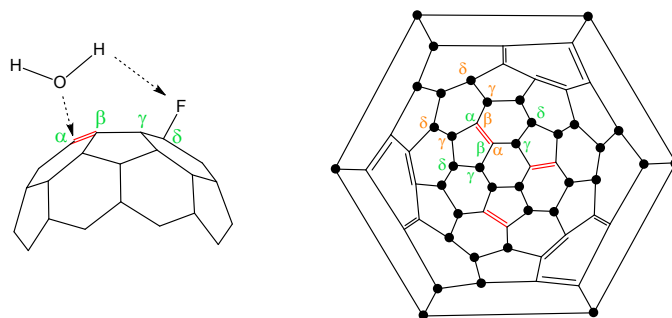


Quantum chemical insights into regioselective hydrolysis of $C_{60}F_{36}$

Ruisheng Zhao^a and Xiang Zhao^{a,*}

S_N2'' mechanism

For S_N2'' mechanism, no channels were located despite much effort has been made. No transition state via S_N2'' mechanism was located but transition state via S_N2' mechanism was gotten during the search of S_N2'' reaction channel, and we think that this is due to that γ -C atom is much more reactive than δ -C atom (Scheme S1).



Scheme S1. Labeling scheme of C_7 isomer for S_N2'' mechanism. Only one isolated double bond was labeled for clarity.

S_N2' mechanism

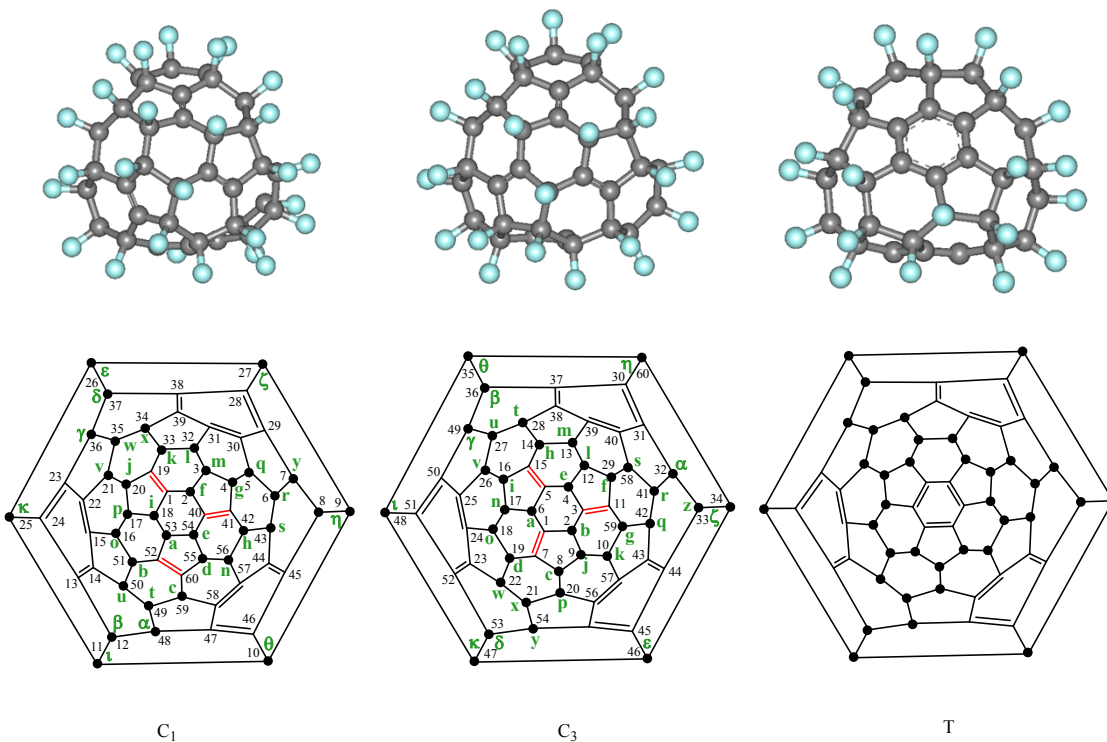


Fig S1. C_1 , C_3 and T isomer of $C_{60}F_{36}$

Table S1. Enthalpy and energy barriers (kcal/mol), H^\ddagger and E^\ddagger , and reaction enthalpies and energies, ΔH and ΔE , of hydrolysis reaction via S_N2' mechanism of C_I isomer in gas phase and in toluene.

		Solution-phase						Gas-phase			
		M06-PCM/6-31G(d)				M06-PCM/6-31+G(d)/M06-PCM/6-31G(d)		H^\ddagger^b	ΔH^b	E^\ddagger^d	ΔE^d
		H^\ddagger^a	ΔH^a	E^\ddagger^c	ΔE^c	E^\ddagger^e	ΔE^e				
C_I -	n=0	25.7		27.2		30.9					
S_N2' -	n=1	10.4	-4.8	11.7	-4.7	15.2	-8.9	28.1	-1.4	29.8	-1.3
$C60-F_a$	n=2	15.8		16.4		20.7					
C_I -	n=0	28.4		29.8		32.7					
S_N2' -	n=1	12.3	7.4	13.5	7.7	16.7	3.9	30.3	10.5	31.1	10.6
$C60-F_b$	n=2	16.1		17.3		21.4					
C_I -	n=0	51.0		52.3		56.4					
S_N2' -	n=1	40.9	22.9	42.1	23.0	45.8	20.3	51.3	24.5	53.5	24.7
$C52-F_c$	n=2	47.3		48.7		52.5					
C_I -	n=0	44.1		45.4		48.8					
S_N2' -	n=1	35.6	19.2	36.9	19.1	40.1	15.0	44.7	20.7	46.7	21.0
$C52-F_d$	n=2	43.6		45.1		48.9					
C_I -	n=0	29.2		30.4		34.9					
S_N2' -	n=1	18.9	3.5	20.6	3.8	22.4	-0.1	31.7	7.1	33.7	7.3
$C40-F_g$	n=2	27.4		28.6		32.7					
C_I -	n=0	32.5		31.3		38.0					
S_N2' -	n=1	19.5	11.4	21.1	11.7	25.3	8.5	35.2	14.3	37.2	14.6
$C40-F_h$	n=2	27.9		29.0		32.2					
C_I -	n=0	41.1		42.4		45.5					
S_N2' -	n=1	33.7	7.6	34.8	7.8	38.5	3.1	42.6	10.1	44.5	10.2
$C41-F_f$	n=2	38.7		40.1		44.6					
C_I -	n=0	40.7		41.7		45.9					
S_N2' -	n=1	30.6	21.9	31.9	22.1	34.6	18.5	41.7	24.5	43.5	24.6
$C41-F_e$	n=2	34.8		36.4		39.5					
C_I -	n=0	31.7		33.1		36.7					
S_N2' -	n=1	25.1	3.3	26.8	3.6	30.4	-0.4	37.2	6.8	39.1	7.1
$C1-F_j$	n=2	39.0		42.1		44.6					
C_I -	n=0	33.7		34.9		39.4					
S_N2' -	n=1	27.4	14.8	28.7	15.1	31.9	11.4	36.0	17.8	37.9	18.1
$C1-F_k$	n=2	35.2		36.8		40.3					
C_I -	n=0	43.6		45.0		48.4					
S_N2' -	n=1	31.6	13.0	32.2	13.0	36.0	8.5	43.6	15.4	45.4	15.5
$C19-F_l$	n=2	36.1		37.7		41.5					
C_I -	n=0	38.3		39.5		42.6					
S_N2' -	n=1	29.5	5.8	31.3	5.7	33.2	1.1	38.8	8.7	40.6	8.8
$C19-F_i$	n=2	34.9		36.4		40.4					

^a These enthalpy values were obtained from frequency calculations at M06-PCM/6-31G(d) level, 25 °C and 1 atm in toluene on the geometries optimized at the same level.

^b These enthalpy values were obtained from frequency calculations at B3LYP/6-31G(d) level, 25 °C and 1 atm in gas phase on the geometries optimized at the same level.

^c These values including corrections for zero-point vibrational energies were obtained from optimization calculations at M06-PCM/6-31G(d) level in toluene, and the scale factor for zero-point energies is 0.980. Zero-point vibrational energies were obtained from frequency calculations at the same level, 25 °C and 1 atm.

^d These values including corrections for zero-point vibrational energies were obtained from optimization calculations at B3LYP/6-31G(d) level in gas phase, and the scale factor for zero-point energies is 0.977. Zero-point vibrational energies were obtained from frequency calculations at the same level, 25 °C and 1 atm.

^e These values were obtained from single-point calculations at M06-PCM/6-31+G(d) level in toluene on those geometries which were optimized at M06-PCM/6-31G(d) level in toluene.

S_N1 and S_N2 mechanism

Table S2. Bond lengths (Å) and energies (kcal/mol) of 36 C-F bond of C_7 isomer

	bond length	bond energy		bond length	bond energy		bond length	bond energy
C10-F _θ	1.38111	288.7	C59-F _c	1.37835	296.7	C54-F _e	1.37204	304.6
C27-F _ζ	1.38085	289.6	C32-F _l	1.37625	297.5	C51-F _b	1.36928	305.5
C25-F _κ	1.38098	289.6	C20-F _j	1.37505	297.6	C42-F _h	1.37007	306.1
C2-F _f	1.38313	292.1	C4-F _g	1.37553	297.9	C33-F _k	1.36895	307.6
C18-F _i	1.37801	293.0	C8-F _z	1.37234	298.9	C17-F _p	1.35825	320.3
C43-F _s	1.37751	294.4	C56-F _n	1.37238	299.1	C9-F _η	1.35764	321.0
C53-F _a	1.37779	294.6	C12-F _β	1.37278	299.5	C11-F _l	1.35734	321.0
C16-F _o	1.37717	294.9	C7-F _γ	1.37264	299.9	C26-F _ε	1.35663	321.7
C5-F _q	1.37670	295.4	C48-F _α	1.37220	300.1	C6-F _r	1.35582	322.5
C34-F _x	1.37689	295.5	C36-F _γ	1.37163	300.8	C35-F _w	1.35512	323.0
C21-F _v	1.37626	295.7	C37-F _δ	1.37146	300.9	C3-F _m	1.35914	324.2
C50-F _u	1.37649	296.6	C55-F _d	1.37135	303.4	C49-F _t	1.35726	324.8

Four C-F bonds with long bond lengths and low bond energies, C10-F_θ, C27-F_ζ, C25-F_κ and C2-F_f, were sifted, and hydrolysis reaction via S_N1 and S_N2 mechanism was investigated on these four bonds.

Table S3. Energy barriers (kcal/mol) of hydrolysis reaction via S_N1 and S_N2 mechanism, E[‡](S_N1) and E[‡](S_N2)

	E [‡] (S _N 1) ^a		E [‡] (S _N 2) ^a
C_7 -S _N 1-C10-F _θ	265.4	C_7 -S _N 2-C10-F _θ	101.5
C_7 -S _N 1-C27-F _ζ	262.9	C_7 -S _N 2-C27-F _ζ	109.7
C_7 -S _N 1-C25-F _κ	267.2	C_7 -S _N 2-C25-F _κ	119.1
C_7 -S _N 1-C2-F _f	265.7	C_7 -S _N 2-C2-F _f	99.5

^a These values including corrections for zero-point vibrational energies were obtained from optimization calculations at B3LYP/6-31G(d) level in gas phase, and the scale factor for zero-point energies is 0.977. Zero-point vibrational energies were obtained from frequency calculations at the same level, 25 °C and 1 atm.

C_3 isomer

Table S4. Enthalpy barriers (H[‡]) and (ΔH) of hydrolysis reaction at B3LYP/6-31G(d) level via S_N2' mechanism of C_3 isomer. All the enthalpies are given in kcal/mol

	H [‡]	ΔH
C_3 -S _N 2'-C1-F _c	29.5	1.4
C_3 -S _N 2'-C1-F _d	32.0	11.3
C_3 -S _N 2'-C7-F _b	42.5	10.2
C_3 -S _N 2'-C7-F _a	44.6	14.7

Regioselectivity

$\langle\Delta H\rangle$ and $\langle H^{\ddagger}\rangle$ were calculated based on the following equation,

$$\langle H \rangle = \sum w_i H_i$$

where w_i and H_i are the weight coefficient enthalpy of isomer i , and was calculated by the following equation,

$$w_i = \{q_i \exp[-\Delta H_{0,i}^{\circ}/(RT)]\} / \sum q_i \exp[-\Delta H_{0,i}^{\circ}/(RT)],$$

where R is gas constant, and T is absolute temperature, and $\Delta H_{0,i}^{\circ}$ is the enthalpy at the absolute zero temperature or ground-state energy (the relative potential energies corrected for the vibrational zero-point energy), and q_i is partition function.¹⁻³

Table S5. Weight coefficients of transition state, w_i (TS), and product w_i (IP), reaction enthalpies (ΔH) and barriers (H[‡]), and mean enthalpy values, $\langle\Delta H\rangle$ and $\langle H^{\ddagger}\rangle$, at M06/6-31G(d) and B3LYP/6-31G(d) level. All the enthalpies are given in kcal/mol.

	M06						B3LYP					
	w _i (TS)	H [‡]	<H [‡] >	w _i (IP)	ΔH	<ΔH>	w _i (TS)	H [‡]	<H [‡] >	w _i (IP)	ΔH	<ΔH>
C _J -S _N 2'-C60-F _a	0.384	10.4		0.572	-4.8		0.266	28.1		0.456	-1.4	
C _J -S _N 2'-C60-F _b	0.616	12.3	11.6	0.428	7.4	0.4	0.734	30.3	29.7	0.544	10.5	5.1
C _J -S _N 2'-C52-F _c	0.326	40.9	38.1	0.478	22.9	21.0	0.526	51.3	48.2	0.598	24.5	23.0
C _J -S _N 2'-C52-F _d	0.647	35.6		0.521	19.2		0.474	44.7		0.402	20.7	
C _J -S _N 2'-C40-F _e	0.708	18.9	19.1	0.331	3.5	8.8	0.395	31.7	33.8	0.441	7.1	11.1
C _J -S _N 2'-C40-F _f	0.292	19.5		0.669	11.4		0.605	35.2		0.559	14.3	
C _J -S _N 2'-C41-F _g	0.196	33.7	31.2	0.111	7.6	20.3	0.803	42.6	42.4	0.369	10.1	19.2
C _J -S _N 2'-C41-F _e	0.804	30.6		0.889	21.9		0.197	41.7		0.631	24.5	
C _J -S _N 2'-C1-F _j	0.179	25.1	27.0	0.278	3.3	11.6	0.286	37.2	36.3	0.379	6.8	13.6
C _J -S _N 2'-C1-F _k	0.821	27.4		0.722	14.8		0.714	36.0		0.621	17.8	
C _J -S _N 2'-C19-F _f	0.403	31.6	30.3	0.502	13.0	9.4	0.610	43.6	41.7	0.636	15.4	13.0
C _J -S _N 2'-C19-F _i	0.597	29.5		0.498	5.8		0.390	38.8		0.364	8.7	

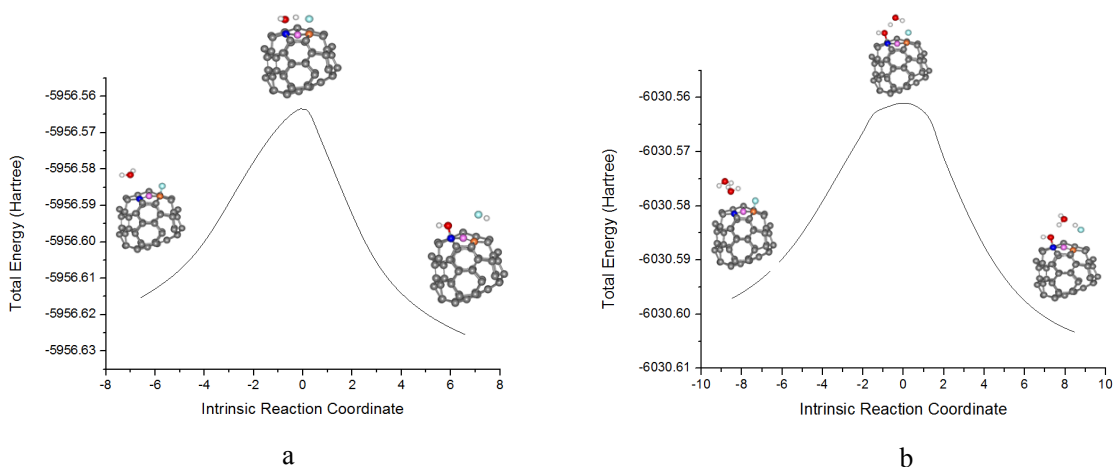


Fig S2. Reaction paths of hydrolysis of C_J isomer via C_J-S_N2'-C60-F_a channel in gas phase (a) and in toluene (b)

References

- 1 S. Miertus, E. Scorocco and J. Tomasi, *Chem. Phys.*, 1981, **55**, 117.
- 2 Z. Slanina, *Int. J. Quantum Chem.*, 1979, **16**, 79
- 3 Z. Slannina, *Int. Rev. Phys. Chem.*, 1987, **6**, 251

Coordinates of structures

B3LYP/6-31G(d) method

C_1 isomer

C	-3.02359100	-0.43928900	-1.02777500
C	-3.28291600	1.01838000	-1.19159200
C	-2.54908400	1.73781800	-2.38430900
C	-1.76112600	2.97051700	-1.64812000
C	-0.28061500	3.24822300	-2.03792300
C	0.72661800	3.88421700	-0.94575500
C	2.15008900	3.07704900	-1.21148200
C	3.03970600	2.58618200	-0.02234500
C	3.96550700	1.21598600	-0.16502100
C	3.77222800	0.48413800	1.25055300
C	3.76016200	-1.08920600	1.36275700
C	2.64147800	-1.69483200	2.42023000
C	1.63476500	-2.27076000	1.49252200
C	0.31755600	-2.54178200	1.79793200
C	-0.55345800	-2.93608800	0.79984100
C	-1.96526500	-3.01484500	1.25620000
C	-2.96821200	-2.61368700	0.09211700
C	-3.59936200	-1.14777100	0.17015600
C	-2.37532600	-1.23797400	-1.86888400
C	-2.35833300	-2.67659300	-1.43491300
C	-0.96010600	-3.32868700	-1.67090000
C	-0.10220000	-3.08006300	-0.48988300
C	1.21711600	-2.81689500	-0.79806600
C	2.07653300	-2.38008400	0.18917500
C	3.47462100	-1.90711700	0.00906700
C	3.67654200	-1.25547900	-1.40800500
C	3.67725100	0.34987300	-1.45223500
C	2.34558600	0.66779800	-2.02921400
C	1.67822300	1.87083900	-1.93727900
C	0.37649800	1.96638400	-2.38256600
C	-0.24697800	0.87362400	-2.93830200
C	-1.68655000	0.76694200	-3.28926700
C	-1.88818300	-0.81421000	-3.21703400
C	-0.45384100	-1.42757200	-3.52915500
C	-0.03324400	-2.81067700	-2.89124700
C	1.50471200	-2.83622000	-2.25443600
C	2.52373600	-1.67688800	-2.52996800
C	1.73535900	-0.42109100	-2.62158200
C	0.43240100	-0.32378900	-3.06338300
C	-2.77775200	1.66888300	0.05965300
C	-1.91368800	2.65435800	-0.18201500

C	-1.30672800	3.53500200	0.85978700
C	0.22001400	3.86100400	0.55250200
C	0.90881300	2.81365500	1.36381600
C	2.13383500	2.22665100	1.10158200
C	2.51934200	1.08835400	1.78489000
C	1.71092200	0.56806700	2.77824900
C	1.88073600	-0.76545900	3.42140500
C	0.32515900	-1.12325900	3.88196300
C	-0.37607700	-2.29821400	3.09121500
C	-1.88749700	-2.15854700	2.59344000
C	-2.24328700	-0.73373500	2.32719800
C	-3.44692600	-0.35810900	1.51196100
C	-3.30374500	1.21890700	1.39108300
C	-2.35119800	1.63997400	2.56698900
C	-1.31389600	2.82177800	2.27795500
C	0.08449400	2.28286900	2.34095900
C	0.49665700	1.16796500	3.05266800
C	-0.44438700	0.27069800	3.78563700
C	-1.67406300	0.31317800	2.92327900
F	-4.64816300	1.20770700	-1.30697800
F	-3.50048700	2.28819200	-3.18380100
F	-2.47015800	4.12106600	-1.90424200
F	-0.28688800	4.08433200	-3.13162700
F	0.92429700	5.18277400	-1.28177900
F	2.91327800	3.87659700	-2.02535700
F	3.88783900	3.60346700	0.33699600
F	5.26377000	1.60623700	-0.23843900
F	4.81298600	0.91384900	2.05033300
F	4.98844600	-1.46257900	1.80352000
F	3.26799100	-2.68203600	3.13956300
F	-2.26079400	-4.31207000	1.61183700
F	-3.99680200	-3.49899600	0.14758000
F	-4.95286600	-1.27167400	-0.05699700
F	-3.26195300	-3.37035500	-2.20493600
F	-1.15137200	-4.68063600	-1.84338500
F	4.30348400	-3.01111600	0.04476300
F	4.88001400	-1.67386000	-1.87388700
F	4.63761300	0.70921600	-2.37707000
F	-1.88153900	1.14695300	-4.59756500
F	-2.78532300	-1.23103700	-4.16329600
F	-0.34740200	-1.56059200	-4.89546600
F	-0.08689300	-3.74314300	-3.87307000
F	2.07299600	-4.02342600	-2.64037800
F	3.18654700	-1.94158800	-3.70108500

F	-2.02124600	4.70291500	0.91026600
F	0.48613900	5.10075300	1.09076000
F	2.62062600	-0.66546300	4.57270500
F	0.36351700	-1.48063000	5.19077100
F	-0.30456000	-3.42298300	3.88147300
F	-2.74992700	-2.66886600	3.52656000
F	-4.56626400	-0.63085400	2.26761300
F	-4.53597800	1.79797500	1.56069700
F	-3.13026400	2.02919000	3.62631200
F	-1.51026400	3.79135300	3.22916700
F	-0.74641500	0.72240200	5.05236100
C ₃ isomer			
C	-2.98903400	-0.50397700	-1.30901300
C	-3.38411400	-1.47618000	-0.22588900
C	-2.98953000	-0.88030500	1.09118700
C	-3.38375200	0.54387600	1.39161300
C	-2.98839600	1.38624100	0.21715200
C	-3.38333000	0.93459400	-1.16636300
C	-2.23417300	-1.05073600	-2.25713900
C	-2.05452200	-2.53884100	-2.09623800
C	-2.68678200	-2.83790700	-0.60941900
C	-1.69856800	-3.39245700	0.50014200
C	-2.23377000	-1.42784400	2.03812300
C	-2.68628000	0.89239000	2.76280200
C	-1.69747600	2.12997600	2.68809400
C	-1.73918100	3.15147100	1.45803600
C	-2.23272200	2.48012700	0.21780200
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C	-2.68544800	1.94758200	-2.15373400
C	-1.69713800	1.26365400	-3.18827700
C	-1.73975000	-0.31232100	-3.45830500
C	-0.59042100	-2.98879000	-2.38403300
C	0.30775900	-2.14981300	-3.42961900
C	-0.23543000	-0.71235700	-3.80048600
C	0.51365200	0.35005600	-3.07328200
C	-0.28871400	1.42644800	-2.74440200
C	0.20457100	2.43897000	-1.95475800
C	-0.58877800	3.55925800	-1.39650200
C	0.30900000	4.04495500	-0.14683500
C	-0.23483700	3.64765900	1.28332200
C	-2.05422600	-0.54508200	3.24675600
C	2.28695500	0.89180800	2.00321200
C	1.49717800	0.08984000	2.80142500
C	1.82176500	-1.29216600	3.23913500

C	2.71838900	-1.92362100	2.12250200
C	3.79273200	-0.99782900	1.25647000
C	3.79323200	1.58514300	0.23539300
C	2.71962100	2.79864200	0.60432400
C	1.80723900	2.10529700	1.54991400
C	0.51387400	2.48661600	1.84038000
C	-0.28914400	1.66379000	2.60773800
C	0.20334900	0.47306800	3.08901600
C	0.30749000	-1.89556900	3.57637300
C	-0.23651100	-2.93525500	2.51696600
C	0.51278700	-2.83753600	1.23330700
C	1.80637100	-2.39556400	1.04883700
C	2.28685700	-2.18193200	-0.22857400
C	3.62933200	-1.54208000	-0.24583500
C	3.79301900	-0.59014400	-1.49103100
C	3.62957500	0.98285500	-1.21136200
C	1.82341900	3.45067600	-0.50083600
C	1.49859600	2.38114400	-1.47936200
C	2.28741600	1.28803600	-1.77431500
C	1.80709800	0.28868800	-2.59816600
C	2.71909100	-0.87732700	-2.72611300
C	1.82211900	-2.15976300	-2.73799900
C	1.49717000	-2.47197100	-1.32243800
C	0.20310100	-2.91235000	-1.13485700
C	-0.28978800	-3.09095000	0.13684100
C	-0.59031000	-0.57004300	3.78016400
C	-1.74060600	-2.83758400	1.99961800
C	3.62931000	0.55636900	1.45793800
F	-4.75552100	-1.65086300	-0.22215000
F	-4.75509600	0.63516200	1.54092400
F	-4.75468200	1.01913000	-1.31981500
F	-2.54699700	4.21852500	1.74375500
F	-1.88165500	2.86638500	3.83616500
F	-3.66199900	1.21804100	3.65101200
F	-2.85867500	-1.02974400	4.25106300
F	-2.54904700	-3.61791500	2.78092600
F	-1.88383200	-4.75475100	0.56397600
F	-3.66259800	-3.76972700	-0.77164800
F	-2.85886900	-3.16681500	-3.01784900
F	-2.54715700	-0.59763300	-4.52574500
F	-1.88103800	1.89032300	-4.39978600
F	-3.66090800	2.55449100	-2.87975900
F	-2.85694400	4.19736000	-1.23375000
F	-0.06327000	4.74240600	2.10057700

F	0.37857200	5.39791400	-0.19157200
F	-0.63404900	4.59678500	-2.30071900
F	-0.06401900	-0.55174600	-5.15726400
F	0.37666300	-2.86490000	-4.57907600
F	-0.63573900	-4.29055300	-2.83051600
F	-0.06630200	-4.19051700	3.05649600
F	0.37607400	-2.53353900	4.77041500
F	-0.63539900	-0.30560500	5.13075200
F	3.43588900	3.78597900	1.23134700
F	2.52239400	4.47407100	-1.08854000
F	3.43475300	-0.82827100	-3.89515300
F	2.52011300	-3.18159800	-3.32976900
F	3.43390000	-2.96042500	2.66467700
F	2.52026900	-1.29408000	4.41966500
F	5.04452900	2.10465700	0.31056300
F	4.57246500	0.92203000	2.39768700
F	5.04395700	-1.32264000	1.66931400
F	4.57258400	-2.53860700	-0.39920700
F	5.04439200	-0.78487600	-1.97833400
F	4.57286700	1.61419800	-1.99749100

C₁-S_N2'-C60-F_a

RC

C	-2.65426000	-1.52715400	0.97793600
C	-2.76580200	-2.35211500	-0.25677700
C	-1.71910900	-3.51585000	-0.42627200
C	-1.04825300	-3.20344700	-1.88658500
C	0.49859700	-3.29581000	-2.03151100
C	1.25393200	-2.36614400	-3.11526300
C	2.64224300	-1.90359300	-2.33231400
C	3.18347200	-0.43960800	-2.43396300
C	4.01926000	0.24844100	-1.17411500
C	3.43933100	1.74372500	-1.11081100
C	3.29002300	2.50862700	0.26121800
C	1.91041300	3.41298900	0.40206800
C	1.11723700	2.60411300	1.36263300
C	-0.25229200	2.65894200	1.52749600
C	-0.87623900	1.73288200	2.34246700
C	-2.35579400	1.80834600	2.28157900
C	-3.02089200	0.38115300	2.45934000
C	-3.54956200	-0.32525300	1.12888700
C	-1.88077400	-1.76267200	2.03258800
C	-2.06895800	-0.76984800	3.14431400
C	-0.70383400	-0.35113300	3.77358400
C	-0.13941800	0.78335900	3.00712700
C	1.22989300	0.73214400	2.85013400

C	1.85179400	1.62216300	1.99884300
C	3.28130200	1.60708400	1.59017500
C	3.86290500	0.14523900	1.59987500
C	3.98821200	-0.57586800	0.17075100
C	2.86032600	-1.54373800	0.18491800
C	2.27650500	-2.14057200	-0.91273600
C	1.12954500	-2.88995400	-0.75427000
C	0.58379500	-3.06447200	0.49616200
C	-0.73327600	-3.67999400	0.80217300
C	-1.05559900	-2.99610200	2.20733500
C	0.36573100	-2.65272400	2.83545000
C	0.52222400	-1.40443800	3.79163700
C	1.85736200	-0.45800400	3.47855500
C	2.98891900	-0.93927900	2.50802800
C	2.33567100	-1.74769100	1.44674900
C	1.18836700	-2.49735600	1.60257300
C	-2.53396500	-1.41299500	-1.40080800
C	-1.57217000	-1.83049200	-2.22346900
C	-1.17537200	-1.14611100	-3.48885600
C	0.40078300	-1.17586000	-3.71306700
C	0.79968800	0.14166500	-3.13641200
C	2.00944500	0.46593900	-2.54884700
C	2.13884100	1.63846600	-1.82819500
C	1.07856500	2.52034800	-1.74315200
C	0.99711400	3.69503800	-0.83297200
C	-0.64815400	3.87118400	-0.64770300
C	-1.22590000	3.50832300	0.78115900
C	-2.55817300	2.63489700	0.93962300
C	-2.74363400	1.72393400	-0.22821300
C	-3.67653100	0.54839700	-0.16503700
C	-3.39661300	-0.19148000	-1.54138400
C	-2.73532400	0.89249200	-2.46804100
C	-1.57182100	0.39071100	-3.44543000
C	-0.27183200	1.01070600	-3.03269800
C	-0.12231000	2.20040300	-2.34275700
C	-1.27045500	3.00630400	-1.83428100
C	-2.27086500	1.94779900	-1.45506400
F	-4.04707900	-2.86925800	-0.32003600
F	-2.41022100	-4.68083900	-0.54097900
F	-1.59211100	-4.09112700	-2.78599700
F	0.81319500	-4.60540600	-2.31717100
F	1.61558700	-3.16068100	-4.15279600
F	3.63125200	-2.76451700	-2.73877500
F	3.98862000	-0.34750000	-3.54140200

F	5.32103200	0.33955000	-1.54868400
F	4.28139200	2.51682400	-1.88641300
F	4.34786500	3.35402000	0.35841300
F	2.27677600	4.61571200	0.95432300
F	-2.80874800	2.59268700	3.32114100
F	-4.09185600	0.55368200	3.27776400
F	-4.81191100	-0.80917300	1.39806600
F	-2.80496800	-1.36960900	4.13942200
F	-0.94029800	0.02846200	5.07559900
F	3.99867100	2.31111700	2.53744100
F	5.11100800	0.21536000	2.12817600
F	5.16618800	-1.29549900	0.20530600
F	-0.58103700	-5.02924900	1.02716400
F	-1.72492500	-3.86566100	3.02595800
F	0.78791500	-3.75976500	3.53726900
F	0.64126700	-1.87530600	5.05702300
F	2.41825400	-0.15063200	4.69196100
F	3.89521000	-1.68211300	3.22049200
F	-1.79697200	-1.77150800	-4.53755900
F	0.61833100	-1.16341500	-5.07312900
F	1.44805800	4.83128600	-1.45848100
F	-0.92234100	5.18206400	-0.88506600
F	-1.42993600	4.69577800	1.45089800
F	-3.66294000	3.42969600	1.09857300
F	-4.96560000	1.03224000	-0.19245100
F	-4.58883300	-0.60000500	-2.08467500
F	-3.71757400	1.43710200	-3.25174700
F	-1.90776300	0.76842200	-4.72187200
F	-1.76826800	3.83559800	-2.81659700
H	-3.92032100	5.22884200	-0.35028900
O	-3.74442800	4.81346400	-1.20695200
H	-3.23528500	5.47204500	-1.70077800
TS	imaginary vibrational frequency -641.08 cm ⁻¹		
C	-2.72033100	-0.98871300	1.43287300
C	-2.98394400	-2.03236800	0.39762800
C	-2.05890100	-3.30927700	0.41806500
C	-1.47406300	-3.37970600	-1.11367000
C	0.04575700	-3.65043300	-1.32158600
C	0.79328400	-3.03617000	-2.61468200
C	2.27587000	-2.57085800	-2.02460900
C	2.92998900	-1.21470600	-2.44977800
C	3.92100500	-0.37907600	-1.41238200
C	3.47671700	1.14944200	-1.62013500
C	3.52017300	2.18475000	-0.43402300

C	2.24646800	3.24671300	-0.40037900
C	1.47896000	2.74872300	0.76975200
C	0.14296300	2.98276200	1.00230300
C	-0.50686600	2.31068000	2.02443400
C	-1.98089900	2.49980000	1.98645000
C	-2.76041300	1.21723400	2.49030800
C	-3.45087600	0.33963600	1.34873000
C	-1.88209600	-1.08360200	2.46047000
C	-1.87865200	0.13055800	3.34526300
C	-0.43552400	0.51807600	3.80812600
C	0.18200700	1.42795500	2.81569800
C	1.52604000	1.19715700	2.59258200
C	2.16547600	1.83411500	1.54838700
C	3.54331900	1.57308400	1.05376000
C	3.97682100	0.08316100	1.32693200
C	3.92166800	-0.91485900	0.07023500
C	2.71422400	-1.73688500	0.34618200
C	1.99950200	-2.48233900	-0.56827300
C	0.80438700	-3.06115900	-0.19412500
C	0.33853900	-2.91790700	1.09205800
C	-1.00099200	-3.31944800	1.59412500
C	-1.15596500	-2.33477700	2.83987200
C	0.33584500	-2.02207500	3.30163300
C	0.68288400	-0.63538300	3.97191200
C	2.07719000	0.08167900	3.40281700
C	3.07559100	-0.69921400	2.48385200
C	2.26827000	-1.62468300	1.64877500
C	1.07249400	-2.20279400	2.01957100
C	-2.74670100	-1.38600400	-0.93475000
C	-1.90160900	-2.06299000	-1.70666000
C	-1.54178900	-1.67881100	-3.10239400
C	0.00702000	-1.90313500	-3.38713500
C	0.55149100	-0.55030400	-3.07804500
C	1.82734000	-0.23957800	-2.65516200
C	2.10977600	1.03276600	-2.19824100
C	1.13754300	2.01359800	-2.22691500
C	1.25261400	3.35942800	-1.60996900
C	-0.34192600	3.75361800	-1.37420600
C	-0.81498600	3.72233200	0.13267800
C	-2.14940400	2.96811900	0.49546400
C	-2.34533300	1.79348700	-0.39397600
C	-3.35376400	0.87679600	-0.07984800
C	-3.47148900	-0.11620300	-1.25500600
C	-2.86712600	0.65753000	-2.48962500

C	-1.78465400	-0.12505500	-3.34264700
C	-0.42997600	0.42349800	-3.07304100
C	-0.13804300	1.70537200	-2.65908100
C	-1.14651900	2.76493600	-2.36732300
C	-2.38777200	2.03710500	-1.82612500
F	-4.30690000	-2.42365900	0.50266100
F	-2.85849000	-4.39494400	0.59081000
F	-2.15563700	-4.37975400	-1.76838800
F	0.22660500	-5.01511400	-1.35034900
F	0.99950700	-4.05096900	-3.49013700
F	3.15116500	-3.58882100	-2.30810100
F	3.64030400	-1.41257500	-3.60717100
F	5.19190500	-0.49442000	-1.87537200
F	4.30206800	1.65863900	-2.60414200
F	4.65770600	2.91051500	-0.58677900
F	2.77331800	4.49091600	-0.15933800
F	-2.33329300	3.54194500	2.81688000
F	-3.75159000	1.65479700	3.31099200
F	-4.76657200	0.13232300	1.68245100
F	-2.59196500	-0.17165200	4.48346900
F	-0.54862600	1.15576400	5.02371500
F	4.41507900	2.36275800	1.77782600
F	5.26326600	0.11452100	1.75860400
F	5.02734300	-1.73532200	0.17838200
F	-0.95159500	-4.60374300	2.08762400
F	-1.83401300	-2.95033300	3.85819900
F	0.70826200	-3.00838700	4.18829700
F	0.85197300	-0.85936500	5.29845900
F	2.75877800	0.54295100	4.50061200
F	3.95979900	-1.38685500	3.27647400
F	-2.28698600	-2.42057200	-3.98044300
F	0.14534700	-2.15746300	-4.73409900
F	1.75836100	4.27018700	-2.50536900
F	-0.52043900	5.01767500	-1.83548600
F	-0.91200600	5.03125300	0.55293000
F	-3.20637200	3.86599900	0.41921200
F	-4.82298200	1.76302600	-0.34619300
F	-4.77155300	-0.46695400	-1.53148000
F	-3.91028900	0.92195000	-3.35962400
F	-2.10709500	0.04362200	-4.67153900
F	-1.48836600	3.46301900	-3.51121000
H	-4.00431000	2.83955400	-2.94276100
O	-3.64434300	2.99355700	-2.04379400
H	-4.33883100	2.56975500	-1.29115300

PC

C	-2.68635800	-1.29177400	1.24584400
C	-2.83357100	-2.28826600	0.13830300
C	-1.81579600	-3.49184600	0.15164100
C	-1.15551200	-3.44827000	-1.35084800
C	0.39104200	-3.58760200	-1.48464100
C	1.15050900	-2.85937000	-2.70730800
C	2.56662500	-2.31789100	-2.02017900
C	3.13723800	-0.89810700	-2.34719800
C	4.01512700	-0.04442800	-1.22457400
C	3.47048900	1.45804800	-1.38833800
C	3.37502300	2.43963300	-0.15950800
C	2.02287400	3.40596300	-0.15051800
C	1.22383600	2.78146000	0.93504900
C	-0.14205000	2.89571700	1.09158800
C	-0.79076400	2.13303900	2.04359400
C	-2.27048700	2.24925200	1.97937500
C	-2.94685800	0.87198500	2.37370200
C	-3.41635900	0.01851700	1.13813500
C	-1.91047100	-1.37371300	2.32147100
C	-2.03956600	-0.18938300	3.24473400
C	-0.65603800	0.28495400	3.78234300
C	-0.07473100	1.26875500	2.83883900
C	1.29152000	1.15236600	2.68489000
C	1.93468600	1.88486300	1.70886100
C	3.35728400	1.75967000	1.29520000
C	3.89239800	0.29570100	1.52936500
C	3.97925800	-0.64647400	0.23159900
C	2.82561700	-1.56876600	0.40575500
C	2.21378400	-2.31968300	-0.57712800
C	1.04572900	-2.99749900	-0.29308900
C	0.50841200	-2.95070100	0.97233100
C	-0.81693800	-3.48041100	1.38437500
C	-1.10386700	-2.58019900	2.67578900
C	0.33622500	-2.16799900	3.21991300
C	0.53803300	-0.78625200	3.96132600
C	1.89225400	0.05854800	3.49025500
C	2.99706800	-0.60424700	2.60199300
C	2.30844700	-1.55102200	1.68672100
C	1.14168700	-2.23130900	1.96827700
C	-2.59643300	-1.56974400	-1.16553400
C	-1.66259900	-2.14581100	-1.91668400
C	-1.25857200	-1.65218900	-3.26742400
C	0.31987800	-1.74765600	-3.46460900

C	0.74125700	-0.38228600	-3.04464000
C	1.97271400	0.00092500	-2.55440200
C	2.14245900	1.26713600	-2.02948400
C	1.10041200	2.17141800	-2.05519100
C	1.09037900	3.50582800	-1.40292000
C	-0.54398900	3.78270000	-1.24457500
C	-1.09196100	3.65504700	0.23229700
C	-2.45864700	2.88044600	0.52015200
C	-2.68246600	1.80933400	-0.49995800
C	-3.14575800	0.59806600	-0.21360700
C	-3.32105900	-0.28209500	-1.42372400
C	-2.80410500	0.56805700	-2.64236100
C	-1.60496500	-0.10008800	-3.43478700
C	-0.31277300	0.51150700	-3.03258900
C	-0.13084800	1.78501600	-2.54570200
C	-1.20218000	2.77775000	-2.31384100
C	-2.55867100	2.07459600	-1.98172200
F	-4.12582800	-2.78088600	0.18141000
F	-2.53643200	-4.64125000	0.23777900
F	-1.71637300	-4.47387600	-2.07578300
F	0.68158900	-4.93176300	-1.56009300
F	1.47348600	-3.81154300	-3.61655200
F	3.52737100	-3.25552500	-2.30288300
F	3.91124100	-0.98305500	-3.47667900
F	5.31192800	-0.04888000	-1.62454800
F	4.30118300	2.07149400	-2.30486900
F	4.46203600	3.25056000	-0.21236300
F	2.43796000	4.66744100	0.19212600
F	-2.70366200	3.18397900	2.89196400
F	-4.04582500	1.16409900	3.11955000
F	-4.79132300	-0.23509200	1.25494700
F	-2.78820800	-0.57547900	4.33148800
F	-0.86689400	0.87672300	5.00763900
F	4.11208700	2.57805400	2.11234600
F	5.14805100	0.40719500	2.03190200
F	5.13755000	-1.38552700	0.36889200
F	-0.68858400	-4.78178400	1.81372900
F	-1.76935200	-3.30185400	3.62956800
F	0.74977000	-3.15647000	4.08460300
F	0.65769000	-1.05128700	5.28543000
F	2.47624900	0.53920900	4.63485000
F	3.88874900	-1.25398000	3.41688700
F	-1.88975200	-2.39628200	-4.22742600
F	0.55968500	-1.91046500	-4.81108600

F	1.57713500	4.47753900	-2.24077900
F	-0.78702700	5.05077800	-1.66011400
F	-1.22856800	4.93536300	0.72139300
F	-3.49118700	3.76869500	0.51159400
F	-4.66309600	-0.58003200	-1.60003500
F	-3.83029100	0.69134400	-3.52994200
F	-1.82496900	0.12669500	-4.77683400
F	-1.41455400	3.50368700	-3.48655900
O	-3.61486500	2.91670100	-2.31849400
H	-3.42573700	3.30148200	-3.19297400
F	-5.64480100	1.98096100	0.09488300
H	-5.80589800	1.14853300	0.49320000
IP			
C	2.97937400	-1.11593300	-0.87723100
C	3.36921100	-1.42472700	0.53583000
C	2.66116500	-2.67008500	1.19648200
C	2.03279700	-2.05953900	2.58609300
C	0.56477100	-2.42729300	2.96020500
C	-0.32568900	-1.37997600	3.80494700
C	-1.84022600	-1.52132000	3.12859400
C	-2.72542200	-0.26226200	2.84544700
C	-3.79770000	-0.23153500	1.57687500
C	-3.62022800	1.24634300	0.97241600
C	-3.77954700	1.53270200	-0.56865700
C	-2.69467100	2.63163200	-1.18247400
C	-1.78832200	1.74615500	-1.95819300
C	-0.49071100	2.04567100	-2.31822800
C	0.30351800	1.07187400	-2.89307500
C	1.71439300	1.49778200	-3.07351200
C	2.69222700	0.26587500	-2.88453800
C	3.38588500	0.21022000	-1.46936800
C	2.21969700	-1.84525900	-1.68874200
C	2.04771600	-1.23551300	-3.05646200
C	0.58287900	-1.35922700	-3.57360600
C	-0.20093500	-0.18783200	-3.11650600
C	-1.49818400	-0.49031800	-2.75759800
C	-2.27955300	0.46890000	-2.14657900
C	-3.62516800	0.26804700	-1.54666200
C	-3.80261200	-1.20779800	-1.02308200
C	-3.64329200	-1.42570500	0.56016000
C	-2.30671500	-2.06700800	0.67966700
C	-1.51876300	-2.12725300	1.81096700
C	-0.22890400	-2.60901300	1.72214100
C	0.26177800	-3.05530300	0.51710600

C	1.66792100	-3.43765600	0.22726000
C	1.71442300	-3.21067700	-1.35498600
C	0.20912200	-3.40243800	-1.84263400
C	-0.32621400	-2.60407800	-3.09762600
C	-1.83543700	-1.93019400	-2.89661500
C	-2.73707100	-2.30517400	-1.67374000
C	-1.82885400	-2.54878400	-0.52360700
C	-0.53913100	-3.03076400	-0.60926900
C	2.98333800	-0.24248100	1.38866700
C	2.22566700	-0.57273200	2.43032000
C	1.73842500	0.40458900	3.44967400
C	0.23073200	0.09818900	3.86541800
C	-0.50844500	0.98993000	2.92854600
C	-1.80291500	0.84215000	2.47571600
C	-2.27457100	1.65004400	1.45949100
C	-1.47531600	2.64888500	0.94209900
C	-1.79153500	3.49287500	-0.23868600
C	-0.27105700	3.98562500	-0.70739400
C	0.26876000	3.29231100	-2.02170700
C	1.77213600	2.76092000	-2.09291800
C	2.26823500	2.37067300	-0.73757600
C	3.00206400	1.28785300	-0.50106200
C	3.39202200	1.13172300	0.94794800
C	2.70513300	2.33153900	1.70131500
C	1.71062600	1.88715900	2.85207000
C	0.30436500	1.96424300	2.38114100
C	-0.18018200	2.79346100	1.39642300
C	0.62224400	3.75368300	0.60952200
C	2.10087700	3.26732400	0.46700600
F	4.73906500	-1.60846400	0.57146500
F	3.62931000	-3.55515300	1.55252700
F	2.83138500	-2.48741500	3.62089000
F	0.59967700	-3.60670700	3.67054300
F	-0.40095900	-1.83668300	5.07909300
F	-2.54782200	-2.38891900	3.92140900
F	-3.43974900	0.03920700	3.97727400
F	-5.05032400	-0.30813300	2.09325900
F	-4.55675200	2.03714400	1.60817600
F	-5.02638000	2.03625900	-0.75276400
F	-3.40200100	3.47158400	-2.00449800
F	1.89673700	1.96725700	-4.35501500
F	3.67027500	0.38891300	-3.82037000
F	4.75845300	0.25182000	-1.63402800
F	2.84620000	-1.92764100	-3.93657000

F	0.62720300	-1.38355100	-4.94984200
F	-4.56542000	0.43551600	-2.54415300
F	-5.05722200	-1.60057800	-1.35960000
F	-4.59585500	-2.35873900	0.91857300
F	1.84145700	-4.78483300	0.45107700
F	2.51512800	-4.14584300	-1.95305700
F	0.02782800	-4.74188400	-2.10656500
F	-0.40116600	-3.47797900	-4.13124800
F	-2.53416100	-2.17304500	-4.05195100
F	-3.46254000	-3.42655300	-1.98659300
F	2.54294800	0.34364800	4.55560800
F	0.05884700	0.54371900	5.15744800
F	-2.47997300	4.62382300	0.12224400
F	-0.32563000	5.32050200	-0.94463200
F	0.09743600	4.19169400	-3.05045800
F	2.57917800	3.73099500	-2.61856300
F	4.76520300	1.22803600	1.08635100
F	3.68597400	3.06345700	2.30116500
F	1.89121900	2.75663300	3.90685500
F	0.67565100	4.97105400	1.29042100
O	2.93391300	4.36568200	0.25543500
H	2.66493500	5.06925600	0.87301500

C₁-S_N2'-C60-F_b

RC

C	-2.65426000	-1.52715400	0.97793600
C	-2.76580200	-2.35211500	-0.25677700
C	-1.71910900	-3.51585000	-0.42627200
C	-1.04825300	-3.20344700	-1.88658500
C	0.49859700	-3.29581000	-2.03151100
C	1.25393200	-2.36614400	-3.11526300
C	2.64224300	-1.90359300	-2.33231400
C	3.18347200	-0.43960800	-2.43396300
C	4.01926000	0.24844100	-1.17411500
C	3.43933100	1.74372500	-1.11081100
C	3.29002300	2.50862700	0.26121800
C	1.91041300	3.41298900	0.40206800
C	1.11723700	2.60411300	1.36263300
C	-0.25229200	2.65894200	1.52749600
C	-0.87623900	1.73288200	2.34246700
C	-2.35579400	1.80834600	2.28157900
C	-3.02089200	0.38115300	2.45934000
C	-3.54956200	-0.32525300	1.12888700
C	-1.88077400	-1.76267200	2.03258800
C	-2.06895800	-0.76984800	3.14431400

C	-0.70383400	-0.35113300	3.77358400
C	-0.13941800	0.78335900	3.00712700
C	1.22989300	0.73214400	2.85013400
C	1.85179400	1.62216300	1.99884300
C	3.28130200	1.60708400	1.59017500
C	3.86290500	0.14523900	1.59987500
C	3.98821200	-0.57586800	0.17075100
C	2.86032600	-1.54373800	0.18491800
C	2.27650500	-2.14057200	-0.91273600
C	1.12954500	-2.88995400	-0.75427000
C	0.58379500	-3.06447200	0.49616200
C	-0.73327600	-3.67999400	0.80217300
C	-1.05559900	-2.99610200	2.20733500
C	0.36573100	-2.65272400	2.83545000
C	0.52222400	-1.40443800	3.79163700
C	1.85736200	-0.45800400	3.47855500
C	2.98891900	-0.93927900	2.50802800
C	2.33567100	-1.74769100	1.44674900
C	1.18836700	-2.49735600	1.60257300
C	-2.53396500	-1.41299500	-1.40080800
C	-1.57217000	-1.83049200	-2.22346900
C	-1.17537200	-1.14611100	-3.48885600
C	0.40078300	-1.17586000	-3.71306700
C	0.79968800	0.14166500	-3.13641200
C	2.00944500	0.46593900	-2.54884700
C	2.13884100	1.63846600	-1.82819500
C	1.07856500	2.52034800	-1.74315200
C	0.99711400	3.69503800	-0.83297200
C	-0.64815400	3.87118400	-0.64770300
C	-1.22590000	3.50832300	0.78115900
C	-2.55817300	2.63489700	0.93962300
C	-2.74363400	1.72393400	-0.22821300
C	-3.67653100	0.54839700	-0.16503700
C	-3.39661300	-0.19148000	-1.54138400
C	-2.73532400	0.89249200	-2.46804100
C	-1.57182100	0.39071100	-3.44543000
C	-0.27183200	1.01070600	-3.03269800
C	-0.12231000	2.20040300	-2.34275700
C	-1.27045500	3.00630400	-1.83428100
C	-2.27086500	1.94779900	-1.45506400
F	-4.04707900	-2.86925800	-0.32003600
F	-2.41022100	-4.68083900	-0.54097900
F	-1.59211100	-4.09112700	-2.78599700
F	0.81319500	-4.60540600	-2.31717100

F	1.61558700	-3.16068100	-4.15279600
F	3.63125200	-2.76451700	-2.73877500
F	3.98862000	-0.34750000	-3.54140200
F	5.32103200	0.33955000	-1.54868400
F	4.28139200	2.51682400	-1.88641300
F	4.34786500	3.35402000	0.35841300
F	2.27677600	4.61571200	0.95432300
F	-2.80874800	2.59268700	3.32114100
F	-4.09185600	0.55368200	3.27776400
F	-4.81191100	-0.80917300	1.39806600
F	-2.80496800	-1.36960900	4.13942200
F	-0.94029800	0.02846200	5.07559900
F	3.99867100	2.31111700	2.53744100
F	5.11100800	0.21536000	2.12817600
F	5.16618800	-1.29549900	0.20530600
F	-0.58103700	-5.02924900	1.02716400
F	-1.72492500	-3.86566100	3.02595800
F	0.78791500	-3.75976500	3.53726900
F	0.64126700	-1.87530600	5.05702300
F	2.41825400	-0.15063200	4.69196100
F	3.89521000	-1.68211300	3.22049200
F	-1.79697200	-1.77150800	-4.53755900
F	0.61833100	-1.16341500	-5.07312900
F	1.44805800	4.83128600	-1.45848100
F	-0.92234100	5.18206400	-0.88506600
F	-1.42993600	4.69577800	1.45089800
F	-3.66294000	3.42969600	1.09857300
F	-4.96560000	1.03224000	-0.19245100
F	-4.58883300	-0.60000500	-2.08467500
F	-3.71757400	1.43710200	-3.25174700
F	-1.90776300	0.76842200	-4.72187200
F	-1.76826800	3.83559800	-2.81659700
H	-3.92032100	5.22884200	-0.35028900
O	-3.74442800	4.81346400	-1.20695200
H	-3.23528500	5.47204500	-1.70077800
TS	imaginary vibrational frequency -762.25 cm ⁻¹		
C	2.70324100	-1.50104800	-0.86366500
C	2.97485100	-2.00748100	0.51077900
C	2.05429800	-3.17482200	1.02606000
C	1.46386200	-2.59119100	2.43896400
C	-0.05538600	-2.75548700	2.73181000
C	-0.80737300	-1.65816800	3.64384900
C	-2.28903000	-1.49001000	2.90513400
C	-2.94810600	-0.08477200	2.71929000

C	-3.93358300	0.23489300	1.41806900
C	-3.49136900	1.70849600	0.96598800
C	-3.52070700	2.15137200	-0.54806600
C	-2.25094200	3.11041200	-1.01713200
C	-1.47264500	2.18097100	-1.87948500
C	-0.13817000	2.30655200	-2.19525700
C	0.52871500	1.27342200	-2.84341300
C	2.02012700	1.44984400	-2.81466000
C	2.77812000	0.05603800	-2.74525600
C	3.45542900	-0.29081800	-1.34328300
C	1.87793200	-2.01924100	-1.76599200
C	1.89438600	-1.28469400	-3.07729000
C	0.46331100	-1.12392400	-3.67858500
C	-0.15415500	0.12923800	-3.18003300
C	-1.49914400	0.00527800	-2.87565000
C	-2.14859800	1.01667200	-2.19955400
C	-3.52864500	0.97681400	-1.64326400
C	-3.96327100	-0.48933500	-1.26742300
C	-3.92260600	-0.87001700	0.29429500
C	-2.71486800	-1.72970000	0.39873300
C	-2.00575300	-2.01961800	1.54650000
C	-0.80814200	-2.69813300	1.45652700
C	-0.33760600	-3.11183400	0.23216400
C	1.00410900	-3.68481000	-0.04562800
C	1.16204400	-3.31742000	-1.59189200
C	-0.32272900	-3.22460300	-2.15146200
C	-0.65805600	-2.23975900	-3.34323400
C	-2.04793900	-1.35056600	-3.13606000
C	-3.05488500	-1.67873200	-1.98162900
C	-2.25948200	-2.17140600	-0.82843700
C	-1.06434100	-2.85218300	-0.91477600
C	2.74142200	-0.85451100	1.44327100
C	1.89224300	-1.14543600	2.42463700
C	1.53074100	-0.20912400	3.52769000
C	-0.02312400	-0.30267700	3.87577500
C	-0.56970600	0.79089600	3.02490800
C	-1.84587200	0.88893200	2.50400800
C	-2.13069500	1.84589300	1.54974700
C	-1.16114700	2.74654900	1.16406100
C	-1.27100100	3.71445200	0.04403200
C	0.31860500	3.97779500	-0.31803100
C	0.82355400	3.31526900	-1.65389300
C	2.07302800	2.39222800	-1.57915100
C	2.34419600	1.76993300	-0.36235700

C	3.48707900	0.83666400	-0.28865300
C	3.48754500	0.42462100	1.21627400
C	2.87513900	1.67180100	1.99028500
C	1.77547500	1.30713200	3.08931700
C	0.41234800	1.67231800	2.61111500
C	0.10937400	2.64940000	1.69209500
C	1.10896700	3.49775100	1.00175300
C	2.37689700	2.63748000	0.81283000
F	4.29926400	-2.40414000	0.57365400
F	2.85463600	-4.23025800	1.33226200
F	2.14189800	-3.21858500	3.45901700
F	-0.23447300	-3.98333600	3.32924600
F	-1.01897600	-2.21221500	4.86321000
F	-3.16211000	-2.30125300	3.58524100
F	-3.66865300	0.21734100	3.84716400
F	-5.20718300	0.31886100	1.87976800
F	-4.32434800	2.58417800	1.63515500
F	-4.66106800	2.86765700	-0.72289300
F	-2.78120500	4.14086700	-1.75257300
F	2.44510200	2.10798600	-3.94293000
F	3.76867000	0.11407500	-3.67450900
F	4.75335800	-0.68490400	-1.58793000
F	2.61892900	-2.03715700	-3.97434900
F	0.59143700	-1.06821400	-5.04859500
F	-4.39365800	1.38844600	-2.63866000
F	-5.24614600	-0.64283700	-1.68400600
F	-5.02990400	-1.66182400	0.52649600
F	0.95918000	-5.05735300	0.04979000
F	1.84738800	-4.30065000	-2.25409600
F	-0.69824500	-4.48807400	-2.55087600
F	-0.82135100	-2.99860100	-4.45538200
F	-2.72444800	-1.39321200	-4.32977500
F	-3.93198300	-2.63608200	-2.42609300
F	2.27193700	-0.51155200	4.63865000
F	-0.16765900	0.02781200	5.20488800
F	-1.78372100	4.91302400	0.47721800
F	0.49636100	5.31847600	-0.43689500
F	1.01251200	4.31879600	-2.57452300
F	3.34925200	3.55553700	-1.79263500
F	4.71180700	1.52939100	-0.48321800
F	4.77272900	0.21972400	1.66681900
F	3.91696600	2.29035400	2.64667500
F	2.09141800	2.01952800	4.22330700
F	1.40239000	4.61024800	1.75836500

H	4.33427400	3.37449400	0.96239900
O	3.50131500	3.70637200	0.56917200
H	3.57651400	3.72050000	-0.57914300
PC			
C	2.50975300	-1.75351100	-0.92590800
C	2.80602400	-2.24638900	0.44536200
C	1.81725600	-3.31715700	1.04042000
C	1.34359900	-2.64283400	2.45388200
C	-0.17093500	-2.66963700	2.82027000
C	-0.78620700	-1.48531200	3.72511100
C	-2.28290300	-1.21079000	3.04526100
C	-2.82234400	0.24145400	2.82923600
C	-3.83716500	0.60517200	1.56193500
C	-3.28432700	2.01542200	1.03279800
C	-3.35253000	2.41295100	-0.49095800
C	-2.02759500	3.24311800	-1.05367200
C	-1.38446800	2.22394100	-1.92573100
C	-0.05975900	2.21830900	-2.29752700
C	0.47816400	1.10770100	-2.94199900
C	1.97685300	1.13750600	-2.92716600
C	2.62645700	-0.29538700	-2.87094700
C	3.35526900	-0.64387300	-1.49424600
C	1.60299600	-2.23426200	-1.77053500
C	1.62153700	-1.56065200	-3.11141600
C	0.18193100	-1.30274600	-3.66673600
C	-0.31264800	0.01725300	-3.20449800
C	-1.64759500	0.02185500	-2.83545300
C	-2.17326600	1.11116700	-2.17111700
C	-3.51900900	1.20789000	-1.54124000
C	-4.05484000	-0.20419000	-1.08865000
C	-3.97397700	-0.53431400	0.48348600
C	-2.84025400	-1.49231000	0.56942500
C	-2.10868300	-1.80882400	1.69648500
C	-0.97671500	-2.58910400	1.57942400
C	-0.59707200	-3.07767700	0.35149100
C	0.67823100	-3.77147600	0.03743800
C	0.79524400	-3.46575700	-1.52318100
C	-0.70118200	-3.27051400	-2.02367300
C	-1.01143800	-2.30555300	-3.23789400
C	-2.31451700	-1.29487100	-3.00719200
C	-3.28533600	-1.49184200	-1.79423600
C	-2.47842100	-2.00884100	-0.65958500
C	-1.35130600	-2.79361800	-0.77184700
C	2.71369700	-1.04763900	1.34100700

C	1.89181100	-1.24015800	2.37094900
C	1.65984300	-0.25108700	3.46233000
C	0.11969500	-0.19736600	3.86786300
C	-0.36272200	0.89563200	2.97963000
C	-1.64670400	1.09422900	2.51645300
C	-1.88621300	2.03734500	1.53687200
C	-0.85625300	2.82488300	1.06986600
C	-0.93934100	3.78156500	-0.06002000
C	0.65234800	3.90402100	-0.49820000
C	1.02872100	3.13483400	-1.81273300
C	2.12997100	2.06530700	-1.71762000
C	2.75520500	1.71684400	-0.59919700
C	3.65314500	0.52284700	-0.48259100
C	3.57921100	0.14773600	1.05567400
C	3.11660200	1.45123100	1.83772500
C	2.01053200	1.21335500	2.95395300
C	0.67576800	1.65942900	2.47977800
C	0.42816100	2.62567100	1.53521300
C	1.45782300	3.39813600	0.80617900
C	2.76906700	2.54845700	0.65694600
F	4.09365900	-2.75081700	0.45878600
F	2.54300800	-4.42488300	1.34685800
F	2.01366700	-3.29163300	3.46526400
F	-0.41948100	-3.85930300	3.46753400
F	-0.98632500	-1.97904300	4.97146300
F	-3.19158800	-1.91381600	3.79434500
F	-3.45232700	0.65468300	3.97525300
F	-5.07466800	0.82129800	2.07464900
F	-3.99255800	2.98626900	1.71353600
F	-4.43350700	3.22125300	-0.63632100
F	-2.50334600	4.29832100	-1.78953100
F	2.45299800	1.77387500	-4.05605700
F	3.56436600	-0.34071900	-3.85284400
F	4.57649200	-1.20070900	-1.80629900
F	2.24077400	-2.40992400	-4.00033400
F	0.25985100	-1.31831200	-5.04088900
F	-4.40018600	1.65935800	-2.50401500
F	-5.36408500	-0.26273700	-1.44168200
F	-5.13308800	-1.21711800	0.79433600
F	0.52459800	-5.13119000	0.18298300
F	1.37279100	-4.51779000	-2.18143700
F	-1.19401300	-4.51303800	-2.35482400
F	-1.28959400	-3.08830500	-4.30941900
F	-3.05025900	-1.33208800	-4.16518700

F	-4.26044400	-2.38731100	-2.15601500
F	2.41727200	-0.58698300	4.55134200
F	0.05095000	0.20515100	5.18283700
F	-1.32817900	5.02490600	0.37545400
F	0.92790500	5.21545400	-0.68479200
F	1.29391800	4.05697200	-2.79587500
F	4.94332900	0.95187500	-0.72155400
F	4.84064300	-0.19294000	1.48413100
F	4.21368800	1.92511900	2.50302000
F	2.37953000	1.95753200	4.05459800
F	1.80514900	4.52284900	1.54811100
O	3.88767800	3.41048800	0.56550800
H	3.92373600	3.94869800	1.37665600
F	3.63329800	4.58001700	-1.75767100
H	3.97157800	4.27549000	-0.92869000
IP			
C	2.80743500	1.52968500	-0.30104600
C	3.28590500	0.62942000	-1.38348600
C	2.59059800	0.78462200	-2.78751300
C	2.06643800	-0.73056600	-3.11319000
C	0.61841200	-0.91491200	-3.65981700
C	-0.18495800	-2.27200500	-3.32665300
C	-1.74394100	-1.74590100	-3.05483500
C	-2.59975700	-2.31751900	-1.87722500
C	-3.74267400	-1.38253400	-1.10740600
C	-3.54185100	-1.74592900	0.44198200
C	-3.78307900	-0.68256300	1.58258600
C	-2.70908500	-0.75841900	2.84871300
C	-1.91646900	0.48666300	2.65212600
C	-0.65251000	0.71640100	3.15093100
C	0.07653800	1.82065200	2.70714600
C	1.53624200	1.67169700	3.01727000
C	2.48445900	2.35737100	1.96455200
C	3.35562500	1.34291900	1.08890600
C	1.97668300	2.55970900	-0.42453400
C	1.76822100	3.31381700	0.85570400
C	0.27813900	3.74175300	1.06332800
C	-0.46746400	2.68016300	1.78577100
C	-1.74495200	2.45905500	1.29776800
C	-2.45340500	1.34830100	1.70676700
C	-3.74454400	0.86145000	1.14554100
C	-3.93179600	1.28848800	-0.36092700
C	-3.68973400	0.14801100	-1.46965900
C	-2.37094400	0.51600900	-2.04888200

C	-1.52328500	-0.30561300	-2.76459300
C	-0.25788500	0.13653600	-3.09157500
C	0.14504200	1.40264100	-2.73738900
C	1.52021300	1.95174200	-2.85381300
C	1.47404300	3.08184600	-1.72982800
C	-0.05573900	3.50046400	-1.61814700
C	-0.64053300	4.01051600	-0.23899500
C	-2.11528300	3.36062100	0.17535000
C	-2.94459000	2.52273000	-0.85442200
C	-1.97926600	1.79910000	-1.72023300
C	-0.71778700	2.24051600	-2.05530100
C	2.98858600	-0.76554500	-0.91947900
C	2.29120900	-1.46338900	-1.81394900
C	1.91465500	-2.89752300	-1.65793700
C	0.42564900	-3.15687400	-2.16760000
C	-0.33640000	-2.97531500	-0.90196200
C	-1.65842900	-2.60424800	-0.76444400
C	-2.15574800	-2.27906500	0.48186300
C	-1.35101500	-2.38714200	1.59386100
C	-1.70685400	-1.95777700	2.96717300
C	-0.21287500	-1.77172200	3.64111400
C	0.25525600	-0.28353600	3.81742100
C	1.54627000	0.14740600	3.11483700
C	2.30649700	-0.64525700	2.37494400
C	3.45454200	-0.15916200	1.54534800
C	3.55513500	-1.24041100	0.39056800
C	2.86451800	-2.56875700	0.92714000
C	1.90770200	-3.29514600	-0.11771100
C	0.47964400	-3.04748900	0.21216000
C	-0.03010900	-2.76315200	1.45537700
C	0.75985400	-2.64504600	2.69868400
C	2.21520000	-2.14829700	2.38749200
F	4.65078600	0.80267500	-1.52329800
F	3.55662800	1.08002700	-3.69731200
F	2.92001200	-1.26980000	-4.04795200
F	0.67365200	-0.79051200	-5.03009000
F	-0.19839500	-3.03015700	-4.45027900
F	-2.43006300	-1.92338400	-4.22921100
F	-3.23837400	-3.45354500	-2.30391500
F	-4.96569800	-1.83978000	-1.47681700
F	-4.40407200	-2.79189000	0.70700100
F	-5.02075000	-0.92462100	2.08549800
F	-3.44910800	-0.69645100	4.00243900
F	1.82001100	2.21161600	4.25825500

F	3.34813400	3.13862800	2.66521200
F	4.64670300	1.82425700	1.06993900
F	2.50309100	4.47602900	0.78137800
F	0.28159700	4.89726700	1.81197700
F	-4.76084700	1.48242900	1.84582800
F	-5.21581400	1.70817400	-0.49504200
F	-4.65136300	0.34523500	-2.44065300
F	1.67675400	2.58086600	-4.06765600
F	2.22749700	4.16386200	-2.09785600
F	-0.28558400	4.48987200	-2.54800600
F	-0.80646000	5.35187800	-0.34789100
F	-2.89320600	4.40195100	0.61654100
F	-3.72024200	3.38298400	-1.59105800
F	2.79019800	-3.67791400	-2.36327200
F	0.34961800	-4.47015000	-2.57430400
F	-2.32902200	-2.97335400	3.65260600
F	-0.24169800	-2.34480000	4.87031700
F	0.34798700	-0.02408600	5.17106800
F	4.59867600	-0.27915900	2.30457500
F	4.88371300	-1.50228000	0.15128200
F	3.86713500	-3.45858800	1.19532900
F	2.17041600	-4.64629800	-0.03841400
F	0.89257200	-3.89967500	3.28218300
O	3.08213900	-2.56617100	3.40289000
H	3.07805400	-3.53932900	3.42203100

C₁-S_N2'-C52-F_c

RC

C	2.60611500	-1.67237900	-0.81667300
C	2.78468200	-2.24703600	0.54554600
C	1.75885400	-3.35693600	0.98543200
C	1.15795200	-2.77292200	2.39244200
C	-0.37815500	-2.83532100	2.63105800
C	-1.08787500	-1.71639700	3.55594400
C	-2.51689100	-1.41052000	2.77001700
C	-3.06563700	0.04593300	2.62059000
C	-3.96961900	0.48204500	1.29714400
C	-3.40802000	1.93799900	0.92283200
C	-3.33538400	2.42718800	-0.57551000
C	-1.97277700	3.28663800	-0.95424500
C	-1.22285200	2.30753200	-1.78222000
C	0.13467900	2.32939500	-2.02489000
C	0.72990600	1.27101400	-2.68549300
C	2.21188700	1.36226600	-2.71245400
C	2.87991400	-0.07635900	-2.64967000

C	3.48066400	-0.52011600	-1.23724500
C	1.78335400	-2.10297200	-1.76697500
C	1.90515100	-1.33828500	-3.05497300
C	0.50575500	-1.04752300	-3.68268400
C	-0.03021600	0.21172100	-3.11810200
C	-1.39004900	0.19094900	-2.88440800
C	-1.97925400	1.22464900	-2.18569900
C	-3.38615900	1.28957900	-1.70905500
C	-3.95322900	-0.14732400	-1.41159100
C	-3.99809500	-0.58308900	0.13302500
C	-2.86257200	-1.53479300	0.24494900
C	-2.21896300	-1.91213400	1.40462100
C	-1.07528400	-2.67957800	1.33323400
C	-0.59126400	-3.08892500	0.11233800
C	0.71465900	-3.75194600	-0.13791500
C	0.95999200	-3.34670800	-1.66190500
C	-0.49387800	-3.12782700	-2.27071400
C	-0.70957000	-2.08517200	-3.43823800
C	-2.03655700	-1.09698400	-3.24247000
C	-3.11376200	-1.38421800	-2.14135100
C	-2.40041400	-1.97554900	-0.98025800
C	-1.25541300	-2.74144400	-1.04934600
C	2.60013200	-1.10901700	1.50158900
C	1.68442000	-1.36058400	2.43605300
C	1.34398900	-0.44905700	3.56801300
C	-0.21774200	-0.43452700	3.87450900
C	-0.65691100	0.75191700	3.08216600
C	-1.89660200	0.95812900	2.50369800
C	-2.07249600	1.97314700	1.58187000
C	-1.02734100	2.82639400	1.28082100
C	-1.00106400	3.80310100	0.15611100
C	0.63093400	3.93733000	-0.14344800
C	1.13174800	3.30653500	-1.50463700
C	2.45835100	2.41999800	-1.55335500
C	2.68890300	1.72645400	-0.25312000
C	3.64585000	0.57988000	-0.13967600
C	3.45459700	0.11634100	1.36388300
C	2.82592600	1.35404400	2.09944800
C	1.72353600	1.05203800	3.21768800
C	0.39883400	1.58876700	2.76561500
C	0.20432700	2.62931200	1.87307300
C	1.31970000	3.31324400	1.15358500
C	2.29253300	2.18867100	0.93167300
F	4.07306100	-2.74207700	0.64257800

F	2.46639200	-4.47829000	1.28460000
F	1.75601100	-3.47221000	3.41516500
F	-0.66433600	-4.06641100	3.17690000
F	-1.39109000	-2.29993600	4.74169300
F	-3.47617500	-2.17922300	3.38057400
F	-3.81522000	0.34604100	3.73030200
F	-5.25194900	0.64175300	1.71325600
F	-4.21829400	2.84377500	1.57897100
F	-4.40443400	3.23941500	-0.77612100
F	-2.37756700	4.35981500	-1.70861100
F	2.61377800	1.93932200	-3.89677000
F	3.90748900	-0.06501100	-3.53854300
F	4.73721100	-1.03819300	-1.46777600
F	2.59777900	-2.11528100	-3.95350900
F	0.67544900	-0.92377200	-5.04303500
F	-4.15784400	1.80119000	-2.73356900
F	-5.22673700	-0.18056200	-1.87885900
F	-5.16799100	-1.29783200	0.29794700
F	0.56554200	-5.11926000	-0.09383300
F	1.59566500	-4.35587300	-2.33412600
F	-0.94034800	-4.34790600	-2.72662700
F	-0.88599700	-2.78938700	-4.58273500
F	-2.66113700	-1.02825400	-4.46172700
F	-4.04644100	-2.25019600	-2.65212700
F	2.02468200	-0.86656100	4.68148500
F	-0.36484900	-0.16686000	5.21755700
F	-1.42976400	5.03941500	0.57009700
F	0.92545800	5.25917400	-0.17190000
F	1.28715400	4.33820300	-2.40127900
F	3.54988100	3.18715900	-1.86077100
F	4.92913100	1.08866100	-0.26929600
F	4.68052800	-0.17558200	1.90966500
F	3.84809100	2.04293400	2.71398300
F	2.12988900	1.66022200	4.37957500
F	1.89102200	4.30960900	1.91000900
H	5.12437100	3.55011200	0.25580500
O	4.50838200	4.15725400	0.69306500
H	4.68242300	4.03033600	1.63746900
TS	imaginary vibrational frequency		-846.80 cm ⁻¹
C	2.73689100	0.51751300	1.51172000
C	2.86203900	1.92933200	1.05613100
C	1.87391100	2.97727000	1.69310600
C	1.14309700	3.63908800	0.38676800
C	-0.39968800	3.83952000	0.40945700

C	-1.24326200	3.78539300	-0.97300600
C	-2.61750100	2.96907700	-0.56257200
C	-3.24331100	1.89863500	-1.51677900
C	-4.06584500	0.60286700	-0.89489300
C	-3.57340600	-0.62638600	-1.80360200
C	-3.41333500	-2.06731600	-1.17820500
C	-2.08036600	-2.88243000	-1.68548900
C	-1.21651200	-2.83855000	-0.47894500
C	0.15081400	-3.01772200	-0.44883300
C	0.84554000	-2.79958900	0.71865400
C	2.31391200	-2.89239400	0.55498900
C	3.06079400	-1.89837600	1.51579600
C	3.58785300	-0.54960800	0.85954700
C	2.01587500	0.08072800	2.53949600
C	2.18993700	-1.38373200	2.81465000
C	0.82162700	-2.06282100	3.13764400
C	0.17666300	-2.45885600	1.86746700
C	-1.19238400	-2.29522200	1.84867500
C	-1.88283900	-2.44965000	0.66390600
C	-3.32281200	-2.16902000	0.42549400
C	-3.83313300	-1.01601100	1.35902800
C	-3.95474200	0.42769100	0.67357200
C	-2.77783300	1.15117100	1.21777200
C	-2.19386800	2.27626700	0.67951100
C	-1.01004400	2.75005500	1.20403400
C	-0.42095300	2.11275800	2.27136300
C	0.93619400	2.37897500	2.81540200
C	1.26637200	0.96967900	3.48162100
C	-0.15264600	0.35226900	3.85574100
C	-0.34792800	-1.21364500	3.86354800
C	-1.74136800	-1.73762000	3.10947600
C	-2.87807900	-0.73884500	2.69753500
C	-2.21285900	0.53339300	2.31711700
C	-1.02277800	1.00290900	2.83479400
C	2.54995100	1.89502100	-0.40031800
C	1.57431600	2.74102200	-0.74124600
C	1.09107000	2.99039600	-2.13232000
C	-0.47720800	3.20484300	-2.22729900
C	-0.94414400	1.83757000	-2.62396000
C	-2.14403400	1.23723900	-2.27094400
C	-2.31164000	-0.12623600	-2.43096700
C	-1.30466000	-0.89570800	-2.99841600
C	-1.22869900	-2.38775400	-2.89718000
C	0.41183200	-2.65432300	-2.88309000

C	1.03658700	-3.30042700	-1.60267400
C	2.47876500	-2.81851000	-1.03301100
C	2.92985100	-1.45105000	-1.59928000
C	3.75588500	-0.44386700	-0.72768500
C	3.33537900	1.00505700	-1.31952600
C	2.47690800	0.69726200	-2.55983800
C	1.40940800	1.75799500	-3.06392700
C	0.07451300	1.07736400	-3.16714600
C	-0.09930400	-0.29376500	-3.34769900
C	1.00699600	-1.23869300	-3.09792600
C	1.89466500	-0.64692300	-2.18900900
F	4.16877200	2.33679700	1.26107900
F	2.62354700	3.95082300	2.27528700
F	1.70991500	4.87692800	0.18537700
F	-0.65552200	5.05549900	1.00249800
F	-1.59982400	5.05859600	-1.27667600
F	-3.57597100	3.91482200	-0.28860100
F	-4.10373200	2.53896700	-2.37520800
F	-5.38390300	0.78958800	-1.16665100
F	-4.50789000	-0.75630400	-2.81258100
F	-4.50461400	-2.78204900	-1.55680300
F	-2.47543900	-4.17346900	-1.94531900
F	2.70668800	-4.16419400	0.92567900
F	4.14605300	-2.56501300	1.99373900
F	4.85905800	-0.34977000	1.36129000
F	2.99075500	-1.53200800	3.92189900
F	1.07152500	-3.17087800	3.91518500
F	-4.03653700	-3.29691500	0.78051800
F	-5.06830400	-1.36685600	1.79776400
F	-5.09052100	1.00928200	1.20237800
F	0.86388500	3.30641200	3.83006500
F	2.01171300	1.13434600	4.61875200
F	-0.48542600	0.81129200	5.11079400
F	-0.40637000	-1.61280300	5.15709400
F	-2.27774800	-2.71573800	3.90717700
F	-3.72567100	-0.57068600	3.76201600
F	1.72466600	4.11623700	-2.59774700
F	-0.70272200	4.07181200	-3.27491300
F	-1.71964000	-2.97603500	-4.03436500
F	0.66871600	-3.48316400	-3.92928000
F	1.12545600	-4.65848400	-1.81291900
F	3.42319700	-3.77259900	-1.37344200
F	5.08377900	-0.63521000	-0.97778700
F	4.48863200	1.67678000	-1.64440700

F	3.37322500	0.56953900	-3.62453200
F	1.81142200	2.25245600	-4.27867500
F	2.09706600	-1.59044500	-4.46489200
H	4.21365700	-2.75409100	-2.72363700
O	3.85085400	-1.85491500	-2.85903100
H	3.12260900	-1.78443800	-3.73761500
PC			
C	2.93519400	-1.24542400	-0.15022800
C	3.05395000	-1.41359100	1.32117000
C	2.19945100	-2.55909000	1.98014700
C	1.34263200	-1.76658800	3.12638900
C	-0.17491400	-2.07533700	3.27515100
C	-1.17903000	-0.92527000	3.81172800
C	-2.53009300	-1.11603800	2.87357300
C	-3.31461200	0.11556100	2.30769700
C	-4.10470200	0.01217400	0.85148000
C	-3.77749000	1.41696200	0.14277300
C	-3.58468500	1.50352800	-1.42628400
C	-2.35081700	2.47872000	-1.92518500
C	-1.34321500	1.48904700	-2.38553000
C	0.01373600	1.71065200	-2.52736600
C	0.85051100	0.65629500	-2.80819700
C	2.28422800	1.02441900	-2.81490600
C	3.17356100	-0.17223500	-2.32343000
C	3.66736100	-0.10717900	-0.81797200
C	2.33313700	-2.07174900	-0.99852000
C	2.48517900	-1.66523900	-2.43550300
C	1.13857800	-1.82728700	-3.20415000
C	0.33502500	-0.60050200	-3.01351400
C	-1.01882200	-0.82471100	-2.88787400
C	-1.85270600	0.21629900	-2.53392600
C	-3.29992300	0.12613900	-2.20633900
C	-3.65084400	-1.26924800	-1.57745000
C	-3.80407900	-1.29679200	0.01846600
C	-2.54221000	-1.94375700	0.46052800
C	-1.98592600	-1.87437800	1.71924000
C	-0.72921300	-2.39741600	1.94029600
C	-0.03943800	-3.00158500	0.91453400
C	1.38279300	-3.43052800	0.94394700
C	1.73489700	-3.38698800	-0.61085100
C	0.34839400	-3.62993900	-1.35299800
C	0.09766500	-2.98738200	-2.77278000
C	-1.39287000	-2.26001200	-2.94360800
C	-2.53247700	-2.46446700	-1.88587600

C	-1.87110100	-2.58767900	-0.56164700
C	-0.61054300	-3.10325300	-0.34034400
C	2.55673400	-0.13131000	1.90075600
C	1.59469200	-0.31576400	2.80638200
C	0.97231500	0.75940600	3.63097400
C	-0.59322300	0.54355600	3.84250900
C	-1.16129200	1.40623800	2.76065600
C	-2.34013700	1.20912300	2.05414100
C	-2.58408300	1.91739400	0.88636600
C	-1.67554100	2.86076600	0.43820200
C	-1.62649500	3.44638600	-0.94049700
C	0.01252200	3.72096400	-1.13554800
C	0.74795900	2.97864400	-2.28131900
C	2.28546400	2.45971800	-2.09216700
C	2.85219900	2.54999600	-0.60997200
C	3.66573100	1.28279800	-0.03284200
C	3.21703200	1.16278900	1.51573400
C	2.27756500	2.36892300	1.81239000
C	1.12311900	2.16072600	2.91467700
C	-0.23206300	2.31723600	2.29911300
C	-0.47865500	3.00435500	1.12700400
C	0.58429900	3.29833000	0.19592300
C	1.79099700	2.77466300	0.42581500
F	4.38961800	-1.59311300	1.63429800
F	3.05558800	-3.39796100	2.62129700
F	1.93317100	-2.03687000	4.33920300
F	-0.29941600	-3.15974500	4.11390100
F	-1.51824200	-1.24767200	5.08464800
F	-3.40497100	-1.89129800	3.59521600
F	-4.25171700	0.49189600	3.23855200
F	-5.43799800	0.00390600	1.11176300
F	-4.83553000	2.25252300	0.43781900
F	-4.73735400	2.01307200	-1.93231000
F	-2.82715600	3.21540400	-2.98269800
F	2.64585800	1.24958100	-4.13113600
F	4.28306400	-0.17824000	-3.11151400
F	4.98926800	-0.51351000	-0.83871100
F	3.40323300	-2.49303600	-3.03542900
F	1.42883500	-2.00769900	-4.53738800
F	-4.00560100	0.20146100	-3.39129100
F	-4.83559300	-1.66384400	-2.10822700
F	-4.84126800	-2.16805100	0.28846600
F	1.47300300	-4.74226600	1.35022000
F	2.61420700	-4.38482000	-0.93653300

F	0.18220700	-4.99029200	-1.48578100
F	0.17953200	-3.98006000	-3.69153700
F	-1.86694300	-2.61479600	-4.18030700
F	-3.23781400	-3.59534100	-2.20796400
F	1.59373600	0.77179300	4.85321900
F	-0.91127200	1.08238700	5.06875500
F	-2.24854500	4.67093200	-0.99338600
F	0.17748600	5.08217800	-1.32448500
F	0.71537400	3.77498300	-3.40286000
F	3.08737900	3.26400800	-2.85280800
F	4.98111600	1.67503000	-0.02888600
F	4.35015200	1.25308700	2.28911200
F	3.07145300	3.39404100	2.27609900
F	1.32149700	3.10469600	3.89197000
F	-0.75484300	5.80640700	1.06704300
O	3.67103700	3.68651200	-0.51646400
H	4.48579700	3.53227200	-1.02516400
H	-0.66204900	6.01027900	0.15631000
IP			
C	2.87511900	0.06375000	1.28550700
C	2.99636000	1.54282600	1.20673200
C	2.10002700	2.38663800	2.18749200
C	1.28364900	3.38118800	1.17800500
C	-0.24419900	3.57846400	1.39407300
C	-1.19792100	3.91286000	0.12980800
C	-2.56126300	3.01910500	0.42006400
C	-3.29998100	2.25248400	-0.72827900
C	-4.10304100	0.83434500	-0.41162900
C	-3.72433300	-0.10265100	-1.66125000
C	-3.53816200	-1.66388700	-1.47160900
C	-2.27019200	-2.32183100	-2.29725800
C	-1.30551200	-2.60795400	-1.20390700
C	0.05878600	-2.78619600	-1.34319000
C	0.85047300	-2.88092400	-0.22230100
C	2.29818400	-2.94843500	-0.52522600
C	3.14154800	-2.26081100	0.60653300
C	3.64844700	-0.78738000	0.30794900
C	2.23373900	-0.63261600	2.21747500
C	2.39302000	-2.11771800	2.06729400
C	1.03532000	-2.84787300	2.30244100
C	0.28357300	-2.86787300	1.02922200
C	-1.07699500	-2.70485000	1.17347600
C	-1.86564200	-2.53414100	0.05410600
C	-3.31353300	-2.19792800	0.02837000

C	-3.71677200	-1.34217000	1.28115400
C	-3.86027700	0.23527000	1.03085700
C	-2.62235800	0.78142600	1.64349000
C	-2.05517200	2.00997500	1.38415800
C	-0.81881500	2.31635600	1.91218600
C	-0.16164500	1.40906700	2.71083500
C	1.24218500	1.51193300	3.18692800
C	1.58565200	-0.02741600	3.42192000
C	0.18544500	-0.71777400	3.73107300
C	-0.04831000	-2.22597700	3.32919100
C	-1.50928200	-2.51774300	2.58070300
C	-2.64953700	-1.44207300	2.55626900
C	-1.98497700	-0.11591000	2.47897800
C	-0.74481000	0.18969700	3.00045900
C	2.55518400	1.89669800	-0.17468300
C	1.59173000	2.81991000	-0.18576800
C	1.01850100	3.44955700	-1.41030300
C	-0.55339300	3.69431000	-1.29808600
C	-1.09392700	2.48224400	-1.98908400
C	-2.28470800	1.81769300	-1.72402400
C	-2.50807200	0.54699700	-2.23327800
C	-1.56293900	-0.05772000	-3.04501300
C	-1.50021800	-1.51668800	-3.38769400
C	0.14956800	-1.75459400	-3.56246900
C	0.84571200	-2.75693100	-2.60433400
C	2.36209600	-2.47906100	-2.06023000
C	2.94155800	-1.03345100	-2.37602600
C	3.70860900	-0.24914000	-1.19321100
C	3.26494100	1.29769300	-1.35580400
C	2.37662000	1.38396200	-2.63157100
C	1.22155100	2.50483800	-2.66135600
C	-0.13124300	1.87260700	-2.76779000
C	-0.35662000	0.59815300	-3.25356500
C	0.71057300	-0.37051800	-3.33399700
C	1.89769800	-0.05056800	-2.81398700
F	4.32538100	1.88315800	1.38515500
F	2.92558500	3.16122700	2.94004400
F	1.87005500	4.62281800	1.26319100
F	-0.40834300	4.58771300	2.31582900
F	-1.54137600	5.22186700	0.21707200
F	-3.46239600	3.86057600	1.02591600
F	-4.21450500	3.10525500	-1.29626600
F	-5.43347800	1.09281900	-0.50187000
F	-4.74584600	0.04653400	-2.57773100

F	-4.67417600	-2.24784600	-1.93318500
F	-2.72625200	-3.48802300	-2.86186800
F	2.66089700	-4.28314700	-0.50978100
F	4.24480800	-3.03574900	0.79193200
F	4.95244000	-0.73908700	0.76658900
F	3.27308100	-2.56696200	3.02231000
F	1.30853700	-4.13071600	2.71926100
F	-4.02250500	-3.37932300	0.12669500
F	-4.91996100	-1.79808300	1.71186600
F	-4.92990200	0.64933100	1.80021600
F	1.28085900	2.13404400	4.41388900
F	2.42188100	-0.17846100	4.49558200
F	-0.03632400	-0.61668900	5.08645600
F	-0.01249000	-2.96267900	4.46586700
F	-2.00527200	-3.67709700	3.11968100
F	-3.40211100	-1.56682400	3.69550500
F	1.64710900	4.65235900	-1.60640700
F	-0.84140500	4.81144300	-2.04948600
F	-2.07518700	-1.76121000	-4.60709400
F	0.36535500	-2.14113700	-4.85673300
F	0.84250500	-3.99635700	-3.20032100
F	3.19474400	-3.36345800	-2.68910300
F	5.03780300	-0.30960600	-1.52694200
F	4.40485900	2.04631900	-1.53021900
F	3.21343900	1.66829500	-3.68803900
F	1.46208600	3.30681400	-3.75093700
O	3.80472600	-1.13077400	-3.47892000
H	4.59102300	-1.64236300	-3.22124100

C₁-S_N2'-C52-F_d

RC

C	2.60611500	-1.67237900	-0.81667300
C	2.78468200	-2.24703600	0.54554600
C	1.75885400	-3.35693600	0.98543200
C	1.15795200	-2.77292200	2.39244200
C	-0.37815500	-2.83532100	2.63105800
C	-1.08787500	-1.71639700	3.55594400
C	-2.51689100	-1.41052000	2.77001700
C	-3.06563700	0.04593300	2.62059000
C	-3.96961900	0.48204500	1.29714400
C	-3.40802000	1.93799900	0.92283200
C	-3.33538400	2.42718800	-0.57551000
C	-1.97277700	3.28663800	-0.95424500
C	-1.22285200	2.30753200	-1.78222000
C	0.13467900	2.32939500	-2.02489000

C	0.72990600	1.27101400	-2.68549300
C	2.21188700	1.36226600	-2.71245400
C	2.87991400	-0.07635900	-2.64967000
C	3.48066400	-0.52011600	-1.23724500
C	1.78335400	-2.10297200	-1.76697500
C	1.90515100	-1.33828500	-3.05497300
C	0.50575500	-1.04752300	-3.68268400
C	-0.03021600	0.21172100	-3.11810200
C	-1.39004900	0.19094900	-2.88440800
C	-1.97925400	1.22464900	-2.18569900
C	-3.38615900	1.28957900	-1.70905500
C	-3.95322900	-0.14732400	-1.41159100
C	-3.99809500	-0.58308900	0.13302500
C	-2.86257200	-1.53479300	0.24494900
C	-2.21896300	-1.91213400	1.40462100
C	-1.07528400	-2.67957800	1.33323400
C	-0.59126400	-3.08892500	0.11233800
C	0.71465900	-3.75194600	-0.13791500
C	0.95999200	-3.34670800	-1.66190500
C	-0.49387800	-3.12782700	-2.27071400
C	-0.70957000	-2.08517200	-3.43823800
C	-2.03655700	-1.09698400	-3.24247000
C	-3.11376200	-1.38421800	-2.14135100
C	-2.40041400	-1.97554900	-0.98025800
C	-1.25541300	-2.74144400	-1.04934600
C	2.60013200	-1.10901700	1.50158900
C	1.68442000	-1.36058400	2.43605300
C	1.34398900	-0.44905700	3.56801300
C	-0.21774200	-0.43452700	3.87450900
C	-0.65691100	0.75191700	3.08216600
C	-1.89660200	0.95812900	2.50369800
C	-2.07249600	1.97314700	1.58187000
C	-1.02734100	2.82639400	1.28082100
C	-1.00106400	3.80310100	0.15611100
C	0.63093400	3.93733000	-0.14344800
C	1.13174800	3.30653500	-1.50463700
C	2.45835100	2.41999800	-1.55335500
C	2.68890300	1.72645400	-0.25312000
C	3.64585000	0.57988000	-0.13967600
C	3.45459700	0.11634100	1.36388300
C	2.82592600	1.35404400	2.09944800
C	1.72353600	1.05203800	3.21768800
C	0.39883400	1.58876700	2.76561500
C	0.20432700	2.62931200	1.87307300

C	1.31970000	3.31324400	1.15358500
C	2.29253300	2.18867100	0.93167300
F	4.07306100	-2.74207700	0.64257800
F	2.46639200	-4.47829000	1.28460000
F	1.75601100	-3.47221000	3.41516500
F	-0.66433600	-4.06641100	3.17690000
F	-1.39109000	-2.29993600	4.74169300
F	-3.47617500	-2.17922300	3.38057400
F	-3.81522000	0.34604100	3.73030200
F	-5.25194900	0.64175300	1.71325600
F	-4.21829400	2.84377500	1.57897100
F	-4.40443400	3.23941500	-0.77612100
F	-2.37756700	4.35981500	-1.70861100
F	2.61377800	1.93932200	-3.89677000
F	3.90748900	-0.06501100	-3.53854300
F	4.73721100	-1.03819300	-1.46777600
F	2.59777900	-2.11528100	-3.95350900
F	0.67544900	-0.92377200	-5.04303500
F	-4.15784400	1.80119000	-2.73356900
F	-5.22673700	-0.18056200	-1.87885900
F	-5.16799100	-1.29783200	0.29794700
F	0.56554200	-5.11926000	-0.09383300
F	1.59566500	-4.35587300	-2.33412600
F	-0.94034800	-4.34790600	-2.72662700
F	-0.88599700	-2.78938700	-4.58273500
F	-2.66113700	-1.02825400	-4.46172700
F	-4.04644100	-2.25019600	-2.65212700
F	2.02468200	-0.86656100	4.68148500
F	-0.36484900	-0.16686000	5.21755700
F	-1.42976400	5.03941500	0.57009700
F	0.92545800	5.25917400	-0.17190000
F	1.28715400	4.33820300	-2.40127900
F	3.54988100	3.18715900	-1.86077100
F	4.92913100	1.08866100	-0.26929600
F	4.68052800	-0.17558200	1.90966500
F	3.84809100	2.04293400	2.71398300
F	2.12988900	1.66022200	4.37957500
F	1.89102200	4.30960900	1.91000900
H	5.12437100	3.55011200	0.25580500
O	4.50838200	4.15725400	0.69306500
H	4.68242300	4.03033600	1.63746900
TS	imaginary vibrational frequency		-781.38 cm ⁻¹
C	2.74700700	0.51987200	1.50580200
C	2.90415600	1.91083800	0.99722300

C	1.93602200	3.00037200	1.59030400
C	1.21997800	3.62842100	0.25543400
C	-0.31790500	3.85585200	0.27226300
C	-1.15754800	3.76647800	-1.10823900
C	-2.55451100	3.00076700	-0.66290600
C	-3.21150500	1.91216000	-1.57267600
C	-4.06523300	0.65791800	-0.89964900
C	-3.60521200	-0.61498800	-1.76179100
C	-3.46893300	-2.04118200	-1.09460400
C	-2.15247600	-2.90638600	-1.58194200
C	-1.27332100	-2.82254300	-0.38844900
C	0.09472500	-3.01338900	-0.36624800
C	0.79655600	-2.77107500	0.79291500
C	2.26188800	-2.91028000	0.63471700
C	3.02315900	-1.90548500	1.57968000
C	3.57333500	-0.58549000	0.89677900
C	2.02066300	0.12959200	2.54683600
C	2.16511900	-1.33159200	2.86332300
C	0.78506700	-1.97043500	3.19850800
C	0.13676000	-2.38419500	1.93497500
C	-1.22868800	-2.19682000	1.91757200
C	-1.92706300	-2.38125000	0.74297500
C	-3.36506700	-2.08755700	0.50773100
C	-3.84961500	-0.89146500	1.40206400
C	-3.94728200	0.53272600	0.67091600
C	-2.75229800	1.25053400	1.18312700
C	-2.14492600	2.34321200	0.60343300
C	-0.94967100	2.80940800	1.10852600
C	-0.37381500	2.19880300	2.19879800
C	0.98732800	2.45829700	2.73443600
C	1.28834200	1.06610600	3.45416300
C	-0.14150900	0.48720300	3.84397700
C	-0.36500600	-1.07552700	3.89949200
C	-1.76589200	-1.59514900	3.16316800
C	-2.88492400	-0.58811500	2.72555200
C	-2.19706300	0.65837800	2.30121000
C	-0.99718100	1.12130000	2.80078800
C	2.59381000	1.83369800	-0.45729500
C	1.63869300	2.68263100	-0.83939600
C	1.16405800	2.86343100	-2.24616400
C	-0.40398200	3.11748000	-2.34120200
C	-0.91137900	1.75095100	-2.67434400
C	-2.12784100	1.19658000	-2.29777800
C	-2.33336300	-0.16717200	-2.39855300

C	-1.34652200	-0.98468600	-2.92794300
C	-1.30187100	-2.47474500	-2.81308300
C	0.33550300	-2.77857000	-2.82797200
C	0.97123100	-3.36250200	-1.51480600
C	2.44254600	-2.90422400	-0.96631800
C	2.90896600	-1.55509900	-1.54484900
C	3.72225100	-0.53262700	-0.67890700
C	3.33633200	0.87598500	-1.34233700
C	2.40340100	0.49949200	-2.48573000
C	1.45088700	1.56094800	-3.12607300
C	0.08090000	0.93793000	-3.18918300
C	-0.14318100	-0.42573300	-3.30532400
C	0.98034900	-1.39995700	-3.22537900
C	1.89577800	-0.78352600	-2.21216500
F	4.21947500	2.29739700	1.18945800
F	2.70306100	3.98083300	2.13660400
F	1.80946800	4.84755400	0.01142600
F	-0.54987100	5.09827300	0.81889900
F	-1.48303300	5.03447800	-1.46386800
F	-3.48311200	3.98421700	-0.42120500
F	-4.05967600	2.54074000	-2.45150600
F	-5.37937800	0.86874800	-1.17188000
F	-4.54320600	-0.75832100	-2.76612700
F	-4.57807200	-2.74467500	-1.44073100
F	-2.57795400	-4.19833900	-1.77911900
F	2.62246000	-4.17704400	1.04954600
F	4.09576400	-2.57853900	2.07744000
F	4.84950400	-0.39370500	1.39185100
F	2.96343100	-1.46315900	3.97418400
F	1.00807600	-3.06294900	4.00575800
F	-4.09365800	-3.18907700	0.91231100
F	-5.08971400	-1.20319700	1.85641200
F	-5.06693200	1.15364800	1.18966800
F	0.93428100	3.42266300	3.71498000
F	2.03529400	1.25747900	4.58573500
F	-0.46823500	0.98999700	5.08367700
F	-0.42775400	-1.43238600	5.20533500
F	-2.31866400	-2.54098400	3.98844600
F	-3.72304000	-0.36883100	3.78845400
F	1.82586100	3.94013300	-2.77915400
F	-0.60857700	3.94952500	-3.42073400
F	-1.82638000	-3.06829700	-3.93392000
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F	4.49206200	1.50610700	-1.73454200
F	3.63195600	0.21033800	-3.72059200
F	1.90911100	1.96496700	-4.34908100
F	1.63572200	-1.56729800	-4.44593500
H	3.91068500	-0.97714600	-3.33927500
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H	4.81831800	-2.11352200	-2.39272200
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C	-1.26514000	-3.49678500	-0.98017800
C	0.27127200	-3.69599100	-1.14736000
C	1.02921600	-3.10808000	-2.45170300
C	2.46380100	-2.54672300	-1.85103500
C	3.08468300	-1.19772800	-2.34571300
C	4.00055900	-0.26782100	-1.32309300
C	3.51216000	1.22956700	-1.63767500
C	3.44809800	2.31766700	-0.49580900
C	2.11664200	3.29097700	-0.55464300
C	1.31388000	2.76010500	0.57394200
C	-0.04852300	2.90318700	0.73642700
C	-0.68069100	2.25296600	1.76989900
C	-2.14458900	2.45276500	1.78752800
C	-2.87618400	1.18161700	2.34985500
C	-3.49872600	0.20045500	1.27380400
C	-1.85747200	-1.05904400	2.45262100
C	-1.95331800	0.18855800	3.28370500
C	-0.54154400	0.66763100	3.73694600
C	0.04026000	1.49952400	2.66273700
C	1.39941900	1.34898900	2.50195200
C	2.02903800	1.95210400	1.43225000
C	3.44534100	1.77739500	1.01984500
C	3.95840400	0.33897400	1.39057800
C	3.98113900	-0.72268500	0.19007900
C	2.80549600	-1.58248600	0.48408600
C	2.14269200	-2.39398200	-0.41044500
C	0.97091400	-3.01614400	-0.03355300
C	0.47438400	-2.84548200	1.23754600
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C	0.37518300	-1.84845600	3.40106400

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C	2.33117000	-1.43885700	1.77401100
C	1.15461600	-2.05675800	2.14733900
C	-2.67669200	-1.58915100	-0.91482900
C	-1.74574500	-2.22844800	-1.63175900
C	-1.33879700	-1.86667100	-3.02833000
C	0.21429200	-2.06058000	-3.31115200
C	0.72800400	-0.66127100	-3.16440400
C	1.97273100	-0.27223800	-2.69216300
C	2.19207400	1.03703500	-2.30617600
C	1.18511400	1.98487600	-2.43934400
C	1.18203200	3.33609500	-1.80399400
C	-0.45226800	3.62628500	-1.61418400
C	-0.98409000	3.66191300	-0.13151100
C	-2.42588800	3.04887400	0.32673100
C	-3.10089900	2.10107900	-0.72985300
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C	-3.38548200	-0.33013800	-1.33944100
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C	-1.64333300	-0.33161000	-3.31745600
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F	1.30919400	-4.15864500	-3.26261000
F	3.38974600	-3.54360100	-2.04094700
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F	4.38668700	1.72730100	-2.58402000
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F	-0.69179100	1.40599500	4.88874200
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F	0.77637500	-0.54714300	5.34231300
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F	3.96778600	-1.01451300	3.42930800
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F	0.33396700	-2.44116800	-4.63028100
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F	-1.76847900	3.13884400	-3.57461600
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C	-3.37436900	1.77191400	-1.31963700
C	-4.11118500	0.61968200	-0.38197400
C	-3.79265100	-0.75259700	-1.15320000
C	-3.55782500	-2.09456500	-0.35601500
C	-2.33088800	-3.03061300	-0.94170900
C	-1.27810300	-2.80931200	0.07943100
C	0.07663400	-3.00019200	-0.09909800
C	0.95002600	-2.63947500	0.89978300
C	2.37024800	-2.84376300	0.54642900
C	3.27962100	-1.75937300	1.22943300
C	3.72110200	-0.54223700	0.31649300
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C	-3.20428000	-1.95632400	1.20697800
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C	-2.37583600	-0.21848000	3.13572600
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C	2.57498800	1.75116100	-1.13027800
C	1.55487500	2.55733700	-1.44674900
C	0.84149500	2.56291200	-2.76552600
C	-0.72234000	2.83170500	-2.64599900
C	-1.27986400	1.44449700	-2.74055100
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C	-1.73629600	-1.29594100	-2.60358100
C	-1.68334900	-2.76385300	-2.33635400
C	-0.06764400	-3.10352500	-2.58583600
C	0.76118100	-3.51816400	-1.31081400
C	2.30196500	-3.05002900	-1.04158900
C	2.79623500	-1.86911600	-1.95306400
C	3.64719800	-0.67985400	-1.26744800
C	3.10457900	0.63781400	-1.99998400
C	1.92366000	0.17102500	-2.78724200
C	0.98245900	1.14636000	-3.47475100
C	-0.38578900	0.55856900	-3.31033700
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F	3.05104400	4.16266600	1.16591600
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F	-0.37499500	5.16510900	0.24154100
F	-1.65141100	4.85592400	-1.84591500
F	-3.46313100	3.96586200	-0.38922700

F	-4.34747400	2.30868200	-2.12623300
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F	-4.70612900	-2.81358300	-0.44335700
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F	2.75952700	-4.05760800	1.08360700
F	4.41284000	-2.39929900	1.62714200
F	5.05515600	-0.31805600	0.60290100
F	3.59660600	-1.04741900	3.53826400
F	1.66816700	-2.60335400	4.05035200
F	-3.86106200	-2.98925700	1.84564600
F	-4.69179700	-0.88711700	2.69795800
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F	1.54726100	3.80798800	3.04688700
F	2.78099100	1.73630100	3.97182000
F	0.38794600	1.57536500	4.88372100
F	0.44921200	-0.81951000	5.27731600
F	-1.61625700	-2.02414800	4.51175100
F	-3.03797400	0.13691200	4.28209700
F	1.40357100	3.53709300	-3.55031400
F	-1.09271800	3.53420200	-3.77260400
F	-2.38343700	-3.46357600	-3.28600300
F	-0.01009600	-4.13768200	-3.46362900
F	0.76197300	-4.89577800	-1.27134300
F	3.11882000	-4.12215900	-1.31545900
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F	4.10354600	1.15314600	-2.80192500
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C₁-S_N2'-C40-F_g

RC

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C	-0.18261600	3.94114200	-0.77531300
C	1.38966100	3.51876600	-1.09418500
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C	3.62716100	2.11653600	-0.15409100
C	3.64900100	1.30354100	1.22894100
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C	3.11165100	-1.13092800	2.31300500
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C	-3.13690200	-1.28913100	1.53865200
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C	0.34655500	1.09192400	3.09791800
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F	-3.94609600	1.45706100	-3.02640700
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F	2.98145500	4.39006100	0.45487600
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F	0.82221700	-3.52706100	-4.03402800
F	3.01289500	-3.32042000	-2.84321700
F	3.56318000	-0.98881100	-3.81949400
F	-3.00111900	3.99182100	1.14392600
F	-0.66285300	4.97873800	1.31488800
F	2.88801500	-0.22386800	4.50847100
F	0.91360900	-1.59315000	5.11676100
F	0.70919100	-3.58479400	3.72953100
F	-1.85262100	-3.43783200	3.43747700
F	-4.13537700	-1.86495700	2.29462700
F	-4.72646600	0.51124700	1.71174800
F	-3.36617100	1.01653900	3.75783800
F	-2.23212400	3.13551100	3.41835100
F	-0.70146100	0.27608300	5.09250400
H	-5.52070700	2.96498400	-0.98727400
O	-5.57818800	2.59751300	-0.09300600
H	-6.12276600	1.80364500	-0.19657100

TS	imaginary vibrational frequency			-705.98 cm ⁻¹
C	-2.78991600	-0.93811600	-0.97537900	
C	-3.39842600	0.40175100	-1.19031900	
C	-2.72534000	1.25360700	-2.33045100	
C	-2.05526700	2.41663700	-1.49003800	
C	-0.80061500	3.13231600	-1.98627800	
C	0.10487600	3.91574100	-0.90367000	
C	1.64461300	3.38533700	-1.19255300	
C	2.61454400	3.04222200	-0.01123500	
C	3.76248700	1.85863500	-0.17251200	
C	3.71589000	1.09205100	1.23829000	
C	3.97539600	-0.46020700	1.33411400	
C	2.98672600	-1.26082200	2.39135300	
C	2.09027200	-1.99768300	1.46372800	
C	0.84207000	-2.49675000	1.77191900	
C	0.04724400	-3.02692500	0.77338600	
C	-1.32901200	-3.34582300	1.23510000	
C	-2.38986400	-3.10564500	0.08243100	
C	-3.25315100	-1.76923200	0.18265700	
C	-2.03448700	-1.60795300	-1.84183100	
C	-1.78571300	-3.03514300	-1.44129700	
C	-0.30446200	-3.44844600	-1.69950100	
C	0.50857400	-3.07618300	-0.52010400	
C	1.75891500	-2.58250700	-0.83137000	
C	2.53545900	-2.01419300	0.15682300	
C	3.82634300	-1.30047200	-0.02721300	
C	3.89935600	-0.60872200	-1.43875800	
C	3.62087000	0.97114500	-1.46891100	
C	2.25620500	1.06438600	-2.05251800	
C	1.39458600	2.13930700	-1.96149500	
C	0.09980500	2.02297100	-2.42615900	
C	-0.32407000	0.83735500	-2.99003200	
C	-1.73347100	0.46131400	-3.28547200	
C	-1.65060600	-1.11906800	-3.20086200	
C	-0.14311200	-1.47667700	-3.54775500	
C	0.51449100	-2.76806300	-2.91879500	
C	2.03471500	-2.53304300	-2.28920000	
C	2.83453000	-1.21393300	-2.56174100	
C	1.84568000	-0.10896000	-2.65512200	
C	0.54803100	-0.23002200	-3.10885000	
C	-3.30178500	1.26931300	0.07900300	
C	-2.10246900	2.06593000	-0.12945100	
C	-1.78210800	3.11855700	0.86948000	
C	-0.38095900	3.78130000	0.59142800	

C	0.50204700	2.89641700	1.40750000
C	1.80251000	2.52884700	1.12459600
C	2.38605900	1.46775700	1.79395500
C	1.68756300	0.80648800	2.78654600
C	2.08297800	-0.48789900	3.40706800
C	0.61103800	-1.11178100	3.86542700
C	0.11973900	-2.38147600	3.06769500
C	-1.39434000	-2.49573400	2.57372800
C	-1.99046100	-1.15040700	2.31534100
C	-3.25523400	-1.00102300	1.52623400
C	-3.49878500	0.58803400	1.46672800
C	-2.51769300	1.16341500	2.59479000
C	-1.68730600	2.49162200	2.30057200
C	-0.21228100	2.21963400	2.38428300
C	0.38921200	1.18598700	3.07572300
C	-0.38897800	0.12950200	3.78328900
C	-1.61124300	-0.02713900	2.91600800
F	-4.74301100	0.19096500	-1.51124100
F	-3.72903200	1.71982900	-3.12891700
F	-3.31020700	3.60974000	-1.66704100
F	-1.09186900	3.98144300	-3.02304300
F	0.06557200	5.23260000	-1.22807600
F	2.25059300	4.33128000	-1.98426500
F	3.27842300	4.19060000	0.34533800
F	4.97260400	2.47070900	-0.25148000
F	4.67974200	1.68706200	2.02912800
F	5.25329800	-0.62140400	1.76447500
F	3.78096600	-2.13184900	3.09613700
F	-1.40328300	-4.67710300	1.57949600
F	-3.25579000	-4.15153900	0.12474300
F	-4.56846100	-2.10652400	-0.07817400
F	-2.57614700	-3.84020900	-2.22838500
F	-0.27720400	-4.81090500	-1.89128400
F	4.83493800	-2.24391700	-0.01040800
F	5.15559500	-0.80655900	-1.91364800
F	4.50471300	1.49819600	-2.39065000
F	-2.05690000	0.78856500	-4.58115800
F	-2.48911900	-1.69666000	-4.11814100
F	-0.05500500	-1.59850900	-4.91678300
F	0.61782600	-3.69057300	-3.90681400
F	2.79767200	-3.60055400	-2.69114800
F	3.53301400	-1.36016400	-3.73383500
F	-2.74918300	4.11598800	0.89269600
F	-0.38547300	5.04775300	1.13593200

F	2.80029000	-0.28439000	4.55971200
F	0.71380700	-1.46839800	5.17148400
F	0.38000300	-3.48492500	3.84899600
F	-2.15424500	-3.15076100	3.50650400
F	-4.27187100	-1.54469300	2.28620900
F	-4.79179000	0.79791100	1.86037300
F	-3.28965900	1.40733800	3.70448100
F	-2.06182100	3.43240000	3.22932000
F	-0.77145300	0.49702500	5.05609600
H	-4.10418000	3.03094400	-0.83068400
O	-4.51271100	2.30182300	-0.07888600
H	-5.29195700	1.82136400	-0.42984000
PC			
C	-2.70133900	-1.01814800	-1.13292400
C	-3.39058800	0.29152300	-1.34997200
C	-2.62397400	1.21214500	-2.35735700
C	-1.95567000	2.21715000	-1.41632700
C	-0.82570800	3.08770400	-1.88379700
C	-0.02337200	3.91007000	-0.77939800
C	1.55934100	3.46683700	-1.01479600
C	2.46983600	3.10987600	0.20092300
C	3.67681100	1.98709300	0.05744900
C	3.58781300	1.16814200	1.43414100
C	3.91795800	-0.37124900	1.49189500
C	2.91780100	-1.25156900	2.47382100
C	2.09879700	-1.98967300	1.47859000
C	0.85984800	-2.54967200	1.70943100
C	0.13465200	-3.07370800	0.65611200
C	-1.24609800	-3.46833900	1.03971700
C	-2.26241200	-3.22204500	-0.15275000
C	-3.18401300	-1.92763300	-0.04273400
C	-1.87098000	-1.62259300	-1.98219700
C	-1.59099600	-3.05892500	-1.63702000
C	-0.08761500	-3.41181800	-1.84382600
C	0.65614200	-3.05437100	-0.61509500
C	1.89661700	-2.49752500	-0.84931200
C	2.60311300	-1.93764100	0.19434800
C	3.87040000	-1.16780600	0.09763100
C	3.98227500	-0.42555900	-1.28624400
C	3.64771800	1.14366000	-1.27841900
C	2.31970200	1.21221800	-1.94539200
C	1.41715200	2.25450300	-1.86649500
C	0.15811300	2.10358800	-2.40979800
C	-0.20535100	0.92505400	-3.03661600

C	-1.60491800	0.49496500	-3.35408100
C	-1.45262400	-1.07940500	-3.31041800
C	0.07846300	-1.37153100	-3.61782000
C	0.75996000	-2.65623800	-2.99845500
C	2.23670600	-2.38499500	-2.28953700
C	2.99817100	-1.03003200	-2.48248000
C	1.97921100	0.04581900	-2.60504000
C	0.71075900	-0.10765400	-3.13499500
C	-3.55526200	1.14847200	-0.03567300
C	-2.40599100	2.12881000	-0.16555400
C	-2.03273600	3.07323900	0.92939400
C	-0.59096000	3.73022700	0.68735200
C	0.27830000	2.81175100	1.48403500
C	1.61063200	2.51113400	1.25706500
C	2.21064900	1.45804000	1.92133900
C	1.50056600	0.73583500	2.86141800
C	1.93183500	-0.55381600	3.46795000
C	0.47175500	-1.25753700	3.83911000
C	0.07654400	-2.51701200	2.97398400
C	-1.40649300	-2.67882800	2.40705400
C	-2.05238500	-1.35241400	2.17158200
C	-3.28690100	-1.23447500	1.33229200
C	-3.61736900	0.33301400	1.33459400
C	-2.70533000	0.92236600	2.51296800
C	-1.92025400	2.30286700	2.30633300
C	-0.44300000	2.07106000	2.40351600
C	0.17614500	1.04709700	3.09779500
C	-0.57959600	-0.05803300	3.75265700
C	-1.75683800	-0.23746600	2.83151300
F	-4.64412700	-0.00040400	-1.84855800
F	-3.54717800	1.87213600	-3.12826100
F	-2.81594400	5.23505100	-1.25728600
F	-1.25262700	3.94792700	-2.89708800
F	-0.10720700	5.22872200	-1.09744900
F	2.15571300	4.48423100	-1.71925300
F	3.05694700	4.26644500	0.65273900
F	4.85968400	2.65461100	0.06816300
F	4.47080400	1.77915200	2.30303900
F	5.18045700	-0.48757100	1.97743100
F	3.71603900	-2.11022400	3.18811900
F	-1.27759300	-4.81467200	1.32628500
F	-3.08227600	-4.30473600	-0.19453500
F	-4.46925900	-2.30191900	-0.38813400
F	-2.31525100	-3.85127200	-2.49777200

F	-0.00041500	-4.76408600	-2.08280400
F	4.91618300	-2.06895300	0.13487600
F	5.26611900	-0.56114000	-1.70585600
F	4.56701300	1.73680900	-2.12157100
F	-1.94701200	0.84708300	-4.63654500
F	-2.23251400	-1.66315900	-4.27452700
F	0.21176900	-1.45652800	-4.98596200
F	0.94911300	-3.53856300	-4.01016500
F	3.06023200	-3.40816800	-2.68783900
F	3.76327400	-1.11725400	-3.61828400
F	-2.98874200	4.03579400	1.05521100
F	-0.60312200	4.97397800	1.27281100
F	2.58464800	-0.34664100	4.65708100
F	0.53300300	-1.65620500	5.13498400
F	0.35416700	-3.63601500	3.72643700
F	-2.17438600	-3.40291300	3.27951400
F	-4.29297000	-1.88776400	2.01987700
F	-4.92582500	0.42389800	1.75249300
F	-3.51946800	1.09758400	3.60471800
F	-2.33018700	3.15945200	3.29844500
F	-1.02008300	0.26007400	5.01878400
O	-4.69664200	1.95521100	-0.13859500
H	-5.47402600	1.42385400	0.10559900
H	-2.33368400	5.29230600	-2.05782400
IP			
C	2.83182800	1.01019700	-0.82744200
C	3.28124700	-0.09367100	-1.72917300
C	2.34109500	-0.27172300	-2.96824400
C	1.52368100	-1.49880900	-2.56319900
C	0.26655200	-1.87324400	-3.29452400
C	-0.64163200	-3.01400000	-2.64586700
C	-2.12811200	-2.30556300	-2.47114100
C	-2.93254100	-2.48164300	-1.14380200
C	-3.93266600	-1.28743700	-0.59049700
C	-3.67279100	-1.28673300	0.99407400
C	-3.73309500	0.04489000	1.83200600
C	-2.57276800	0.16842900	3.00635300
C	-1.66319600	1.18466100	2.41852200
C	-0.34202300	1.38065300	2.76135200
C	0.43575500	2.25893000	2.03079900
C	1.87311500	2.21524900	2.40790700
C	2.80169300	2.46343500	1.14608200
C	3.49019100	1.17611500	0.50951500
C	2.09648600	2.06439100	-1.17924600

C	2.07580800	3.15782100	-0.14721000
C	0.65049000	3.76780700	0.00691400
C	-0.11195700	2.94810900	0.97526500
C	-1.43347400	2.75509000	0.63012400
C	-2.19959100	1.85106600	1.33485400
C	-3.58204900	1.41556000	1.00909800
C	-3.85275900	1.48750400	-0.54064100
C	-3.79276200	0.09701800	-1.33852100
C	-2.51498000	0.19085800	-2.09665300
C	-1.80501300	-0.86134800	-2.64214000
C	-0.55436100	-0.63204200	-3.18230500
C	-0.00791900	0.64075900	-3.17590700
C	1.43948400	0.97790400	-3.37844800
C	1.55864100	2.32079000	-2.55064700
C	0.09394800	2.93219200	-2.51057600
C	-0.34207700	3.81280400	-1.27228800
C	-1.82419300	3.42592800	-0.63444900
C	-2.81011500	2.46828600	-1.38479300
C	-1.99542100	1.47187000	-2.12936800
C	-0.73380800	1.69620000	-2.64996800
C	3.32422200	-1.50523700	-1.02694200
C	2.01464100	-2.11006000	-1.48775000
C	1.51146400	-3.41724300	-0.97708800
C	-0.02208300	-3.66582500	-1.34635700
C	-0.69720100	-3.17097400	-0.11365000
C	-1.96093100	-2.61531100	-0.02538500
C	-2.35476600	-1.96708900	1.12928400
C	-1.50824100	-1.91993400	2.22089800
C	-1.69669700	-1.05979400	3.42202300
C	-0.12866200	-0.84211200	3.93049300
C	0.45482800	0.61364900	3.75627500
C	1.92928300	0.83273400	3.18708100
C	2.33289700	-0.27135900	2.26503500
C	3.50753500	-0.11954600	1.34917600
C	3.56418000	-1.50498300	0.54821200
C	2.59318400	-2.47625700	1.37460100
C	1.58060400	-3.45076200	0.60159400
C	0.16596500	-3.10224300	0.96564600
C	-0.25105400	-2.48664800	2.13266600
C	0.69926200	-1.96830800	3.15693900
C	1.86481300	-1.51427200	2.31878900
F	4.55487600	0.23001100	-2.15130600
F	3.11567400	-0.59093600	-4.05395600
F	0.56701700	-2.20631800	-4.59797500

F	-0.77386800	-4.00237100	-3.56760500
F	-2.90589900	-2.75410200	-3.51026000
F	-3.69624000	-3.61830300	-1.25430100
F	-5.21119700	-1.70437900	-0.78143400
F	-4.62620500	-2.12338400	1.54097500
F	-4.94511200	0.07504900	2.44268100
F	-3.19440600	0.65557000	4.12927800
F	2.14414600	3.21620400	3.31345600
F	3.79352300	3.29848100	1.55188400
F	4.81153000	1.49451800	0.25635800
F	2.90471400	4.16659900	-0.58127000
F	0.79032300	5.05555300	0.47056600
F	-4.45495600	2.31219200	1.59314000
F	-5.10454200	1.98876800	-0.69941300
F	-4.82345500	0.13735900	-2.25707800
F	1.69705100	1.27284600	-4.69412000
F	2.40407600	3.19680800	-3.18066600
F	-0.05395300	3.71043600	-3.63741500
F	-0.40279500	5.09953000	-1.69502700
F	-2.47101500	4.61150300	-0.38818700
F	-3.57667800	3.21742400	-2.24181700
F	2.28053100	-4.42567400	-1.49372700
F	-0.19732700	-5.02822400	-1.44930000
F	-2.34552000	-1.74112000	4.42083400
F	-0.08787000	-1.14178700	5.25350400
F	0.39141900	1.23090400	4.98525600
F	2.83023100	0.90998200	4.21525500
F	4.62814100	-0.04220000	2.15521100
F	4.84721900	-1.97138900	0.72300600
F	3.39162100	-3.28348800	2.14679900
F	1.87302500	-4.73675700	0.98292800
F	1.11439000	-2.93104900	4.05109100
O	4.29923500	-2.30774200	-1.63779300
H	5.16615200	-2.08280100	-1.25809200

C₁-S_N2'-C40-F_h

RC

C	-2.75983400	-1.15714400	-1.00375600
C	-3.37598600	0.19560800	-1.09945000
C	-2.86690300	1.12131600	-2.26511600
C	-2.38527500	2.47534300	-1.48588800
C	-1.02606600	3.12107200	-1.88181700
C	-0.18261600	3.94114200	-0.77531300
C	1.38966100	3.51876600	-1.09418500
C	2.39810500	3.21234200	0.06010100

C	3.62716100	2.11653600	-0.15409100
C	3.64900100	1.30354100	1.22894100
C	4.02388900	-0.22822500	1.27045100
C	3.11165100	-1.13092800	2.31300500
C	2.25632400	-1.90011900	1.37270900
C	1.05096300	-2.49484100	1.68059600
C	0.28025000	-3.04827300	0.67571300
C	-1.05910900	-3.48822400	1.14525900
C	-2.15492500	-3.29740400	0.01288500
C	-3.12023900	-2.03523000	0.16530400
C	-1.95814900	-1.73844100	-1.88957500
C	-1.58318900	-3.14643500	-1.52259500
C	-0.07475200	-3.42767800	-1.80482900
C	0.72357900	-3.02504200	-0.62446300
C	1.93281900	-2.43727100	-0.93569100
C	2.68209400	-1.84505800	0.06036900
C	3.91706400	-1.03595100	-0.11488100
C	3.92134800	-0.29790600	-1.50351500
C	3.52999000	1.25887100	-1.47561600
C	2.14836100	1.26497000	-2.02200400
C	1.21022700	2.26339100	-1.86685600
C	-0.08504900	2.05453300	-2.29029500
C	-0.43665000	0.86814500	-2.89032000
C	-1.81561900	0.42873200	-3.22728500
C	-1.62280400	-1.15545200	-3.22423000
C	-0.08979600	-1.38727000	-3.58283200
C	0.66900200	-2.65049400	-3.01170500
C	2.18244300	-2.32513300	-2.39519500
C	2.88087000	-0.94201500	-2.63073600
C	1.80855500	0.08578200	-2.65718600
C	0.51132400	-0.12032400	-3.07911400
C	-3.02616500	0.90184900	0.17332300
C	-2.42390900	2.07187400	-0.03471300
C	-2.03156200	3.03477500	1.03599400
C	-0.63488500	3.73402000	0.72580100
C	0.30665800	2.85454500	1.47980000
C	1.63176000	2.59638500	1.17656200
C	2.29864300	1.56033800	1.80321900
C	1.66370300	0.81873000	2.78172100
C	2.16907500	-0.45660300	3.36282200
C	0.75890000	-1.20269400	3.82609500
C	0.34800200	-2.48019300	2.99167400
C	-1.16202700	-2.69371300	2.51819500
C	-1.85999500	-1.38900600	2.32113600

C	-3.13690200	-1.28913100	1.53865200
C	-3.39416800	0.27917600	1.48943900
C	-2.54365000	0.87395900	2.67067400
C	-1.83160900	2.28374100	2.42028200
C	-0.34200800	2.09937700	2.44162700
C	0.34655500	1.09192400	3.09791800
C	-0.32989200	-0.03645600	3.80271800
C	-1.55328600	-0.26034700	2.95911400
F	-4.74866600	0.02300200	-1.20958700
F	-3.94609600	1.45706100	-3.02640700
F	-3.34921300	3.43931700	-1.69822900
F	-1.25826300	3.97086100	-2.94066900
F	-0.31629200	5.26058400	-1.05749300
F	1.91527300	4.51283800	-1.88170300
F	2.98145500	4.39006100	0.45487600
F	4.78950700	2.81452800	-0.22617600
F	4.57064100	1.94161400	2.03593000
F	5.31605500	-0.30648300	1.67969000
F	3.97661200	-1.96199000	2.98103000
F	-1.02083600	-4.83187200	1.44506800
F	-2.93537400	-4.40921800	0.04010000
F	-4.40818700	-2.47576000	-0.05586200
F	-2.30921100	-4.00609500	-2.31324000
F	0.06460200	-4.77759200	-2.03495600
F	4.99148900	-1.90307600	-0.13850400
F	5.17952100	-0.39071300	-2.00286900
F	4.35293200	1.87906000	-2.39459100
F	-2.13070200	0.80389000	-4.51347400
F	-2.41451300	-1.74109200	-4.17563900
F	0.01315400	-1.43524100	-4.95503600
F	0.82221700	-3.52706100	-4.03402800
F	3.01289500	-3.32042000	-2.84321700
F	3.56318000	-0.98881100	-3.81949400
F	-3.00111900	3.99182100	1.14392600
F	-0.66285300	4.97873800	1.31488800
F	2.88801500	-0.22386800	4.50847100
F	0.91360900	-1.59315000	5.11676100
F	0.70919100	-3.58479400	3.72953100
F	-1.85262100	-3.43783200	3.43747700
F	-4.13537700	-1.86495700	2.29462700
F	-4.72646600	0.51124700	1.71174800
F	-3.36617100	1.01653900	3.75783800
F	-2.23212400	3.13551100	3.41835100
F	-0.70146100	0.27608300	5.09250400

H	-5.52070700	2.96498400	-0.98727400
O	-5.57818800	2.59751300	-0.09300600
H	-6.12276600	1.80364500	-0.19657100
TS	imaginary vibrational frequency		-752.26 cm ⁻¹
C	-2.78681800	-0.91553800	-1.04430000
C	-3.42420900	0.43064500	-1.24973600
C	-2.72233500	1.29902800	-2.38195100
C	-2.11222400	2.53933200	-1.56098800
C	-0.75904800	3.15114800	-1.97047400
C	0.09162200	3.92592400	-0.84287600
C	1.64314900	3.41147500	-1.10392600
C	2.59253300	3.06457800	0.08642600
C	3.75031900	1.88639600	-0.07694600
C	3.68040800	1.09853700	1.31659800
C	3.95297000	-0.45409600	1.38732200
C	2.95688000	-1.28058700	2.41132700
C	2.08169100	-2.00893200	1.45702700
C	0.83411800	-2.52447500	1.73703200
C	0.05706800	-3.03962800	0.71640200
C	-1.32415400	-3.37647800	1.14784600
C	-2.37080400	-3.11123200	-0.01871000
C	-3.24553700	-1.78378500	0.09314500
C	-2.00573900	-1.56838800	-1.90428600
C	-1.74758200	-3.00207200	-1.52668100
C	-0.26081400	-3.41012800	-1.76781900
C	0.53627100	-3.05949600	-0.57065700
C	1.78987500	-2.55683000	-0.85305400
C	2.54787700	-2.00126000	0.15754200
C	3.83697500	-1.27551000	0.00988500
C	3.93182600	-0.56265700	-1.38776600
C	3.64384800	1.01569200	-1.39196400
C	2.28935900	1.10548200	-1.99249400
C	1.42027000	2.16966700	-1.88856400
C	0.13531200	2.04625400	-2.36919300
C	-0.28428600	0.87732800	-2.95964400
C	-1.68884300	0.51653800	-3.30461400
C	-1.60085900	-1.06330200	-3.25064400
C	-0.08261800	-1.41409900	-3.57642600
C	0.57315000	-2.71201300	-2.96230100
C	2.08711400	-2.48189000	-2.30578300
C	2.88638200	-1.15524600	-2.54054300
C	1.89070000	-0.05682700	-2.62506200
C	0.59734100	-0.17902500	-3.09434600
C	-3.31327200	1.25221500	0.05564400

C	-2.09927300	2.03704900	-0.15306500
C	-1.76457100	2.94839700	0.84743800
C	-0.45159100	3.76050300	0.63401100
C	0.45446300	2.90122400	1.48118700
C	1.76122800	2.53839900	1.20474900
C	2.33979800	1.46169900	1.85869000
C	1.63602400	0.77510400	2.82831700
C	2.03412800	-0.53077300	3.42582500
C	0.56541400	-1.17717400	3.85247000
C	0.09560700	-2.44011700	3.02508500
C	-1.40901100	-2.56104300	2.50618300
C	-2.00548800	-1.21620100	2.26343200
C	-3.25778400	-1.06033800	1.45710600
C	-3.49513600	0.51375900	1.42444100
C	-2.55265400	1.08061800	2.57654800
C	-1.74761700	2.41645600	2.29773700
C	-0.26435300	2.19018600	2.43591000
C	0.33241800	1.14242600	3.11210000
C	-0.44316000	0.05667200	3.78170800
C	-1.64344500	-0.10199500	2.89043200
F	-4.74489800	0.21515300	-1.58236000
F	-3.71012400	1.75271500	-3.20137100
F	-3.03868600	3.57968400	-1.72085600
F	-0.95135400	4.01686500	-3.02380200
F	0.05456700	5.25137600	-1.13085600
F	2.25374800	4.37193700	-1.87433900
F	3.24650900	4.21027000	0.46853400
F	4.95731000	2.50816400	-0.12148000
F	4.62438400	1.68547600	2.13773200
F	5.22531500	-0.60880400	1.83670800
F	3.74578800	-2.15718500	3.11561500
F	-1.39914100	-4.71587600	1.45742100
F	-3.23114800	-4.16316200	-0.01009900
F	-4.55680900	-2.12556100	-0.17766500
F	-2.52008000	-3.79694800	-2.34244500
F	-0.23183300	-4.77027100	-1.97854900
F	4.85239900	-2.21138000	0.03511100
F	5.19654300	-0.74646100	-1.84489000
F	4.54094400	1.56715400	-2.28585800
F	-1.95773300	0.86959700	-4.60768600
F	-2.41976100	-1.63046000	-4.19168900
F	0.03275700	-1.50692300	-4.94565900
F	0.69536300	-3.61890500	-3.96246400
F	2.85844700	-3.54077900	-2.71403700

F	3.60575800	-1.27599900	-3.70255700
F	-3.10585600	4.04686800	0.92902200
F	-0.57012600	5.01151200	1.18991700
F	2.73370500	-0.34104600	4.59187700
F	0.65408400	-1.55666100	5.15312900
F	0.35638500	-3.55273900	3.79243600
F	-2.17925300	-3.23667100	3.41498500
F	-4.27744100	-1.62809100	2.19693700
F	-4.81199500	0.70052900	1.82564700
F	-3.34217300	1.30780300	3.67944100
F	-2.17894100	3.36879900	3.18620200
F	-0.85546900	0.39093600	5.05453100
O	-4.47070800	2.31577700	0.03743800
H	-3.96437400	3.24808700	0.45269000
H	-5.20809900	1.99786400	0.60007200
PC			
C	-2.71878600	-1.10511500	-0.94301800
C	-3.44943900	0.17597600	-1.19520700
C	-2.85230800	1.05485200	-2.37588100
C	-2.36419700	2.43727100	-1.65071700
C	-0.97282700	3.04015500	-2.03633900
C	-0.11830700	3.88081700	-0.95181700
C	1.44040300	3.43439700	-1.22972100
C	2.44202800	3.19055000	-0.05078000
C	3.65227400	2.06451300	-0.20566000
C	3.66015100	1.32030500	1.21551700
C	4.00804100	-0.21538000	1.32442500
C	3.07379100	-1.05682800	2.39175900
C	2.21971300	-1.85831300	1.47826500
C	1.00779100	-2.42997600	1.80073800
C	0.24202800	-3.02270600	0.81464500
C	-1.11082600	-3.41717900	1.28673900
C	-2.19069300	-3.24643700	0.13549000
C	-3.12598100	-1.96022300	0.22373200
C	-1.93632100	-1.75159500	-1.80478100
C	-1.60117700	-3.15789900	-1.38864700
C	-0.10132600	-3.49490600	-1.64946600
C	0.69831900	-3.06232100	-0.48067000
C	1.91681300	-2.50201400	-0.80576200
C	2.66131900	-1.87081700	0.17026500
C	3.90694100	-1.08378200	-0.02665500
C	3.93332300	-0.41048500	-1.44618000
C	3.55547000	1.14749500	-1.48855800
C	2.17970600	1.13909700	-2.04673500

C	1.25119100	2.15008500	-1.94493500
C	-0.04084100	1.94462500	-2.38252300
C	-0.39873000	0.74161400	-2.94005600
C	-1.77958000	0.30340000	-3.27652200
C	-1.60187700	-1.27030100	-3.17870200
C	-0.07258300	-1.54598100	-3.52198600
C	0.66647600	-2.78873500	-2.88329000
C	2.17943100	-2.45662400	-2.26683900
C	2.89676100	-1.09477500	-2.55643600
C	1.83517800	-0.05920800	-2.64097800
C	0.54157700	-0.26448800	-3.07510900
C	-3.55480100	1.09802000	0.06815600
C	-2.46390600	2.10655500	-0.18656700
C	-1.80043800	2.75823800	0.75385800
C	-0.61001300	3.68469900	0.52050300
C	0.36644100	2.97936000	1.42081100
C	1.67970700	2.67332100	1.12098600
C	2.32191400	1.64241500	1.79117300
C	1.66687300	0.95101100	2.79186100
C	2.13547600	-0.32457600	3.40589900
C	0.70797900	-1.03009400	3.87655500
C	0.29068900	-2.34187800	3.10042200
C	-1.21482000	-2.55849800	2.61745900
C	-1.88607000	-1.25527600	2.33767700
C	-3.16720200	-1.19573100	1.56191100
C	-3.52375700	0.36411900	1.49520600
C	-2.54430900	1.01935000	2.58084000
C	-1.81428800	2.36470600	2.21846200
C	-0.31126700	2.26507700	2.41132500
C	0.34995600	1.26342900	3.09668500
C	-0.36542800	0.14680200	3.78625000
C	-1.56340300	-0.10009800	2.90823000
F	-4.73945600	-0.20255200	-1.54992200
F	-3.88766200	1.37742000	-3.19661300
F	-3.30342200	3.39069200	-1.95377400
F	-1.16248100	3.85556400	-3.12899100
F	-0.23109400	5.19861800	-1.25473800
F	1.98339700	4.38258600	-2.06312900
F	3.04676500	4.38477300	0.25353900
F	4.82430500	2.74373300	-0.30432500
F	4.60125900	1.97702700	1.98500700
F	5.29458400	-0.29534300	1.75157200
F	3.91942100	-1.87151600	3.10457800
F	-1.10651500	-4.74708400	1.64219900

F	-2.99507700	-4.33993700	0.19505200
F	-4.41956100	-2.37618800	-0.02916100
F	-2.34755100	-4.01507400	-2.16404900
F	-0.00096500	-4.85660100	-1.82103400
F	4.97155000	-1.96273300	0.00137900
F	5.19549000	-0.53667100	-1.92773000
F	4.38927000	1.71996000	-2.42898500
F	-2.06156600	0.60821900	-4.58858500
F	-2.40635900	-1.91231500	-4.08095600
F	0.03221300	-1.66556800	-4.88922600
F	0.81791100	-3.71619900	-3.85985100
F	2.99996600	-3.48161600	-2.66331000
F	3.59199600	-1.20273100	-3.73350100
F	-3.54401300	4.92202300	0.90904300
F	-0.87935700	4.95437200	1.05065700
F	2.84857200	-0.07496300	4.55234200
F	0.83896400	-1.36100400	5.18686000
F	0.62763100	-3.41341100	3.89607000
F	-1.92836100	-3.24180000	3.56483000
F	-4.12260700	-1.82437000	2.33830400
F	-4.79708300	0.47124800	1.98181200
F	-3.27962500	1.26168400	3.71644000
F	-2.35111000	3.38362700	2.97913000
F	-0.78776100	0.48177800	5.05502500
O	-4.73170100	1.85502100	-0.02961900
H	-5.47743200	1.24055400	-0.15014200
H	-2.74754500	5.31838600	1.20157200
IP			
C	2.93455400	0.19301200	0.96963500
C	3.41956600	1.39991700	0.22971800
C	2.69795700	2.75566100	0.63469900
C	1.94188700	3.24133000	-0.73110000
C	0.47058400	3.76803300	-0.63476000
C	-0.55426600	3.56949100	-1.86892500
C	-1.99180600	3.22591800	-1.15092600
C	-2.96027300	2.14479800	-1.73876800
C	-3.93243600	1.26086300	-0.72280300
C	-3.83647700	-0.22864900	-1.30999100
C	-3.89274700	-1.48103500	-0.35124700
C	-2.84509000	-2.69265200	-0.74298200
C	-1.83340800	-2.57835300	0.33900300
C	-0.54506700	-3.06598800	0.29437500
C	0.34248000	-2.76094900	1.30922900
C	1.73363400	-3.19355400	1.01545900

C	2.79080100	-2.17121600	1.61578000
C	3.46543000	-1.15949700	0.58664800
C	2.31133500	0.18539900	2.14650200
C	2.23436700	-1.17398800	2.78693400
C	0.83073000	-1.43960100	3.41395200
C	-0.06548800	-1.99160800	2.37207800
C	-1.35838900	-1.51172800	2.42736600
C	-2.23200500	-1.78059400	1.39293000
C	-3.59722100	-1.22146000	1.20935700
C	-3.71381800	0.21051400	1.84543200
C	-3.63291400	1.43904400	0.81808300
C	-2.26614500	1.97076000	1.04674700
C	-1.54676600	2.76764900	0.18625000
C	-0.22894300	3.06608100	0.46381000
C	0.36167100	2.58730300	1.60723800
C	1.80742700	2.65872400	1.94724300
C	1.92617400	1.40674400	2.91494200
C	0.48395100	1.23723700	3.56685000
C	-0.02436900	-0.19757700	3.99397500
C	-1.58805400	-0.54640600	3.53237000
C	-2.54026600	0.56462800	2.97322100
C	-1.68922500	1.51882800	2.21744000
C	-0.36965100	1.81415800	2.49147000
C	3.32173800	1.26290400	-1.32926300
C	2.07059800	2.04616200	-1.63715400
C	1.26030200	1.81683800	-2.65770400
C	-0.06934000	2.51938100	-2.92590700
C	-0.92271800	1.27908300	-3.01123500
C	-2.14591600	1.08393800	-2.39831000
C	-2.59792800	-0.20253700	-2.14167800
C	-1.85058900	-1.29373200	-2.53996200
C	-2.08616400	-2.70211300	-2.10984300
C	-0.56475500	-3.35712400	-2.21127500
C	0.11062500	-3.76665500	-0.84154200
C	1.64128900	-3.41994900	-0.55263100
C	2.06125600	-2.18502700	-1.27652600
C	3.32863600	-1.47106200	-0.91631000
C	3.38888500	-0.22711400	-1.92359100
C	2.27413300	-0.57995800	-3.01956700
C	1.31592100	0.56518100	-3.51145100
C	-0.14812700	0.17888200	-3.38979000
C	-0.62442700	-1.09860600	-3.15898200
C	0.27053600	-2.29158800	-3.05457100
C	1.51356100	-1.74566800	-2.40389200

F	4.76579100	1.51482900	0.55733600
F	3.67482000	3.66520000	0.89607600
F	2.69557900	4.26791300	-1.24857600
F	0.53329800	5.11652800	-0.36394300
F	-0.68654000	4.76131700	-2.50243700
F	-2.68318500	4.40985800	-1.05256500
F	-3.78778200	2.75697600	-2.64674000
F	-5.20878300	1.68240100	-0.91823700
F	-4.90355100	-0.36714600	-2.17679400
F	-5.15211500	-1.98181200	-0.43622500
F	-3.54084200	-3.87219100	-0.63266400
F	1.97297600	-4.41429600	1.60468400
F	3.78475600	-2.92036500	2.16098400
F	4.82042700	-1.13890200	0.85996700
F	3.14773000	-1.20444100	3.81560900
F	0.99394500	-2.34693900	4.43567000
F	-4.47917200	-2.02422100	1.90516400
F	-4.91785400	0.27764800	2.46768600
F	-4.53354200	2.38148700	1.27451500
F	2.05906000	3.78665300	2.69464800
F	2.85855700	1.62788100	3.89227400
F	0.43733000	2.03817500	4.68532300
F	0.02661100	-0.25934500	5.34690600
F	-2.19205600	-1.14521600	4.60856800
F	-3.17297300	1.17553800	4.02514200
F	-0.01217200	3.14590200	-4.15732100
F	-2.86169800	-3.36382400	-3.02964700
F	-0.66314200	-4.48297600	-2.96394900
F	-0.03769200	-5.12831200	-0.70292300
F	2.44760600	-4.46066000	-0.92718500
F	4.36489500	-2.33075400	-1.22934900
F	4.60562300	-0.31253400	-2.54226400
F	2.92202300	-1.05949600	-4.13349600
F	1.65328600	0.89747600	-4.80677900
F	0.59588500	-2.82931000	-4.28155400
O	4.34164100	2.03351100	-1.91096800
H	5.19156300	1.74968800	-1.52967900
C ₁ -S _N 2'-C41-F _f			
RC			
C	-2.75992600	-1.15693200	-1.00372300
C	-3.37611000	0.19583500	-1.09934500
C	-2.86694100	1.12161700	-2.26495600
C	-2.38515800	2.47548100	-1.48565300
C	-1.02599100	3.12125900	-1.88163700

C	-0.18246500	3.94119800	-0.77506300
C	1.38977000	3.51874500	-1.09399400
C	2.39825400	3.21223400	0.06022300
C	3.62724000	2.11638600	-0.15407500
C	3.64910000	1.30330900	1.22891700
C	4.02392300	-0.22846400	1.27031500
C	3.11168500	-1.13120300	2.31285300
C	2.25629500	-1.90030300	1.37253700
C	1.05091000	-2.49497700	1.68042500
C	0.28013700	-3.04831000	0.67553500
C	-1.05922900	-3.48823100	1.14508800
C	-2.15506800	-3.29728300	0.01277000
C	-3.12030500	-2.03507800	0.16529200
C	-1.95825900	-1.73818600	-1.88958500
C	-1.58335600	-3.14622500	-1.52272700
C	-0.07496500	-3.42754900	-1.80502500
C	0.72341800	-3.02500900	-0.62465800
C	1.93265700	-2.43724900	-0.93588600
C	2.68202200	-1.84517600	0.06018600
C	3.91701400	-1.03610500	-0.11506400
C	3.92127600	-0.29797500	-1.50364600
C	3.52996000	1.25878800	-1.47561800
C	2.14831800	1.26497100	-2.02196200
C	1.21025100	2.26343800	-1.86674500
C	-0.08502200	2.05471700	-2.29024700
C	-0.43670000	0.86839900	-2.89038300
C	-1.81571100	0.42902100	-3.22723500
C	-1.62295000	-1.15516000	-3.22422300
C	-0.08997300	-1.38703600	-3.58294100
C	0.66881600	-2.65031400	-3.01188300
C	2.18224000	-2.32506100	-2.39539000
C	2.88073000	-0.94198200	-2.63090400
C	1.80846300	0.08586900	-2.65726800
C	0.51122200	-0.12011900	-3.07923700
C	-3.02615200	0.90198300	0.17347900
C	-2.42373000	2.07193100	-0.03450600
C	-2.03134700	3.03477000	1.03624300
C	-0.63471500	3.73402600	0.72607500
C	0.30685200	2.85449100	1.48000800
C	1.63192100	2.59626600	1.17669300
C	2.29877100	1.56014000	1.80325700
C	1.66384800	0.81850700	2.78174400
C	2.16918000	-0.45689200	3.36273600
C	0.75895900	-1.20294700	3.82601200

C	0.34799300	-2.48038500	2.99153200
C	-1.16205700	-2.69381300	2.51808600
C	-1.85996400	-1.38905400	2.32112700
C	-3.13689500	-1.28908900	1.53869800
C	-3.39410900	0.27924800	1.48959500
C	-2.54350500	0.87392000	2.67081300
C	-1.83141600	2.28368400	2.42048000
C	-0.34181400	2.09928300	2.44181600
C	0.34672400	1.09175500	3.09801600
C	-0.32976000	-0.03665700	3.80272000
C	-1.55318200	-0.26044300	2.95913800
F	-4.74871600	0.02327300	-1.20946400
F	-3.94610900	1.45746100	-3.02622100
F	-3.34907300	3.43960900	-1.69783400
F	-1.25823700	3.97113800	-2.94036800
F	-0.31606000	5.26066700	-1.05716500
F	1.91540100	4.51282700	-1.88150900
F	2.98166700	4.38991500	0.45501900
F	4.78962300	2.81431500	-0.22617500
F	4.57078900	1.94130800	2.03590300
F	5.31610200	-0.30681500	1.67949900
F	3.97664200	-1.96232700	2.98079800
F	-1.02101100	-4.83190500	1.44480300
F	-2.93555100	-4.40907000	0.03992300
F	-4.40831100	-2.47551200	-0.05586900
F	-2.30947400	-4.00577900	-2.31340800
F	0.06431500	-4.77744600	-2.03524400
F	4.99141400	-1.90325600	-0.13877400
F	5.17942900	-0.39081400	-2.00304900
F	4.35285400	1.87903300	-2.39463400
F	-2.13093000	0.80421000	-4.51338100
F	-2.41474700	-1.74074300	-4.17561000
F	0.01285600	-1.43498700	-4.95515100
F	0.82196700	-3.52684400	-4.03425200
F	3.01265400	-3.32039000	-2.84344100
F	3.56301300	-0.98875900	-3.81966500
F	-3.00093100	3.99177300	1.14427100
F	-0.66263900	4.97871300	1.31520600
F	2.88815500	-0.22428000	4.50838000
F	0.91369600	-1.59347500	5.11665100
F	0.70917600	-3.58503600	3.72931300
F	-1.85266500	-3.43795400	3.43733700
F	-4.13535200	-1.86493200	2.29466700
F	-4.72641400	0.51129600	1.71201400

F	-3.36596200	1.01646600	3.75803300
F	-2.23191700	3.13543000	3.41857900
F	-0.70133800	0.27580300	5.09254400
H	-5.52150300	2.96408100	-0.98775300
O	-5.57763900	2.59718000	-0.09318100
H	-6.12330700	1.80385300	-0.19530000
TS	imaginary vibrational frequency		-771.53 cm ⁻¹
C	-2.82606200	-1.17331300	-1.04780800
C	-3.13338800	0.25295300	-1.04338100
C	-2.83637800	1.12910000	-2.26845700
C	-2.44194100	2.55767700	-1.55574800
C	-1.01303100	3.12290700	-1.86332400
C	-0.18771300	3.93518700	-0.76282200
C	1.38885600	3.50857600	-1.07226200
C	2.38351600	3.19226900	0.08474300
C	3.61386100	2.09414600	-0.12610700
C	3.61724900	1.27411700	1.25107100
C	3.99102200	-0.25846000	1.28854900
C	3.07150600	-1.16223700	2.32202800
C	2.21776200	-1.92461700	1.37410600
C	1.00787000	-2.51448500	1.67280800
C	0.23497000	-3.05201300	0.66045500
C	-1.10431300	-3.49874000	1.12031700
C	-2.20105300	-3.30321100	-0.01772300
C	-3.16093900	-2.03931000	0.13756300
C	-2.03110400	-1.76405100	-1.94478100
C	-1.63323300	-3.16143300	-1.56057400
C	-0.11090300	-3.42452700	-1.82342600
C	0.68022000	-3.02039000	-0.63780000
C	1.89875800	-2.44563200	-0.93851100
C	2.64885800	-1.86431500	0.06387700
C	3.89057700	-1.06236100	-0.09912300
C	3.91089900	-0.31968000	-1.48376700
C	3.52615600	1.24040400	-1.45190100
C	2.14713600	1.25133800	-2.00216300
C	1.20818100	2.24749000	-1.83412400
C	-0.08849200	2.03269700	-2.24193800
C	-0.43193400	0.85724900	-2.86179400
C	-1.80086400	0.44321700	-3.23160600
C	-1.64296500	-1.14937700	-3.25358700
C	-0.09874800	-1.38520700	-3.58750500
C	0.64716900	-2.65311800	-3.02186100
C	2.16173500	-2.33588700	-2.39506000
C	2.87460500	-0.95623200	-2.62037400

C	1.80778500	0.07577200	-2.64484900
C	0.50966600	-0.12991400	-3.06275100
C	-2.73827400	0.86253800	0.15187700
C	-2.78641200	2.29414200	-0.04879000
C	-2.12697300	3.12946800	1.06836400
C	-0.65744600	3.71900800	0.72086800
C	0.26085900	2.80417700	1.45559500
C	1.59554200	2.56008300	1.17545100
C	2.25843600	1.52578800	1.80641600
C	1.61784000	0.78519800	2.78113100
C	2.12529800	-0.48770200	3.36769000
C	0.71845100	-1.23590700	3.82806100
C	0.30548100	-2.51088100	2.98392000
C	-1.20411700	-2.72219500	2.50678400
C	-1.88997900	-1.41398200	2.32023200
C	-3.14285600	-1.27812300	1.50404100
C	-3.29379500	0.27963400	1.41873500
C	-2.56000400	0.84882900	2.65513100
C	-1.87448900	2.26630400	2.42373400
C	-0.39047400	2.05838600	2.41474000
C	0.29960900	1.05810900	3.08950200
C	-0.36619300	-0.06768400	3.81177000
C	-1.58485400	-0.29149100	2.97296600
F	-4.89926000	0.48408000	-1.00279400
F	-3.94760700	1.36515900	-3.02201800
F	-3.31847600	3.51848100	-2.03666100
F	-1.15508600	3.96128500	-2.95310200
F	-0.32272000	5.25712500	-1.04207200
F	1.91717300	4.50036700	-1.85937700
F	2.96406800	4.36283400	0.50442700
F	4.77809600	2.79002200	-0.18397300
F	4.52759800	1.90709100	2.07507200
F	5.28133600	-0.33804100	1.70436400
F	3.93094700	-1.99667700	2.99322300
F	-1.06068400	-4.84645100	1.40417800
F	-2.98375300	-4.41394700	0.01488600
F	-4.45271000	-2.47652900	-0.05564500
F	-2.33075700	-4.05738500	-2.33684500
F	0.04216700	-4.77538100	-2.04625000
F	4.96119100	-1.93469300	-0.11608900
F	5.17225900	-0.41536300	-1.97437900
F	4.35780300	1.86166900	-2.36210400
F	-2.08660500	0.85239700	-4.51473300
F	-2.40904800	-1.69243400	-4.25064500

F	0.02605200	-1.41621500	-4.95906600
F	0.80179000	-3.52688000	-4.04658500
F	2.98870400	-3.33605700	-2.83861900
F	3.56446600	-1.00174400	-3.80471900
F	-2.93012000	4.19589000	1.35286100
F	-0.60655100	4.95746200	1.32836300
F	2.84142700	-0.24911200	4.51445600
F	0.87472000	-1.63569800	5.11596500
F	0.67088900	-3.61856700	3.71540100
F	-1.89533100	-3.47719500	3.41690500
F	-4.18037500	-1.78998600	2.25669500
F	-4.64210400	0.58678900	1.56268500
F	-3.43701800	0.97711200	3.70272300
F	-2.23341400	3.08022400	3.47047400
F	-0.72233800	0.25384500	5.10413200
H	-4.55402100	3.38499600	-0.58049000
O	-4.37369200	2.61454600	-0.00244400
H	-4.80267400	1.67557300	-0.45181900
PC			
C	-2.63838500	-1.14550700	-0.99089900
C	-2.77362200	0.26883700	-1.08371200
C	-2.65111600	1.00720700	-2.37871800
C	-2.32847800	2.52059900	-1.86324300
C	-0.85405000	3.00843500	-2.15206600
C	-0.02751500	3.87236600	-1.08972100
C	1.54197100	3.37698700	-1.31054800
C	2.48804800	3.11987000	-0.09670600
C	3.69006200	1.97720900	-0.17645300
C	3.62539300	1.26811700	1.26227400
C	3.94673700	-0.26617600	1.43486200
C	2.96235800	-1.05760700	2.50357400
C	2.11633200	-1.86521500	1.58747600
C	0.87969200	-2.39614100	1.88754800
C	0.12934500	-2.99933200	0.89538200
C	-1.23702300	-3.36793800	1.34527600
C	-2.28422700	-3.23867700	0.16324200
C	-3.16268100	-1.91584800	0.17936600
C	-1.95755300	-1.87583300	-1.87600900
C	-1.66304900	-3.26010900	-1.38105900
C	-0.13522800	-3.56969200	-1.56787000
C	0.62031500	-3.08815900	-0.38563300
C	1.86093400	-2.56195700	-0.68664000
C	2.59296300	-1.92211400	0.29310800
C	3.86439600	-1.17222900	0.11053800

C	3.95272700	-0.54049400	-1.32713100
C	3.61548100	1.02617500	-1.43281600
C	2.25644600	1.03524100	-2.03362200
C	1.34315700	2.06873100	-1.98314100
C	0.05422400	1.86498200	-2.42722300
C	-0.29437600	0.65837100	-2.98846000
C	-1.67474800	0.24829600	-3.33122400
C	-1.54149000	-1.35823500	-3.21969200
C	-0.00278400	-1.65676500	-3.49280800
C	0.68485800	-2.89828100	-2.79570400
C	2.17891900	-2.57299500	-2.13674300
C	2.93707600	-1.23515100	-2.44535400
C	1.90499800	-0.17764000	-2.59441300
C	0.62231400	-0.37326600	-3.06068300
C	-2.93233000	1.03699300	-0.00839400
C	-2.85440000	2.50179700	-0.33500000
C	-2.02985200	3.30660200	0.74380100
C	-0.53660700	3.79031400	0.39079200
C	0.31250600	2.89120000	1.21549000
C	1.64762000	2.59337700	1.00977400
C	2.25720900	1.59982800	1.74788200
C	1.55821100	0.95831500	2.75334000
C	2.00241500	-0.27565800	3.45978700
C	0.55334800	-0.94085100	3.92300200
C	0.13060200	-2.26345500	3.16675900
C	-1.36753500	-2.46566900	2.65419300
C	-2.01446000	-1.15487000	2.34421700
C	-3.23855300	-1.06634500	1.48240000
C	-3.41221500	0.50319000	1.30488100
C	-2.63279700	1.15150100	2.49015700
C	-1.86816600	2.52107300	2.15949600
C	-0.39588200	2.24908300	2.20754600
C	0.23864700	1.29105000	2.98587500
C	-0.49247200	0.25609800	3.77268400
C	-1.69757600	0.00757700	2.91425100
F	-5.63997300	0.07807500	-1.00430400
F	-3.88181000	1.03922300	-2.98364700
F	-3.14662100	3.38383500	-2.53505600
F	-0.91815800	3.77345700	-3.30190400
F	-0.10953500	5.17371900	-1.47075500
F	2.13299000	4.28831000	-2.14865400
F	3.08814200	4.30198900	0.25787200
F	4.87657900	2.63285000	-0.24761400
F	4.52750900	1.93867600	2.06429100

F	5.21844500	-0.35249700	1.90215400
F	3.77032600	-1.86297200	3.26722700
F	-1.24685600	-4.68405900	1.75158000
F	-3.12319000	-4.30111300	0.26721500
F	-4.45378200	-2.27897100	-0.13170900
F	-2.36195300	-4.20057000	-2.09238700
F	0.00222500	-4.93401900	-1.68713100
F	4.90517900	-2.07581000	0.19741100
F	5.22698300	-0.71027500	-1.76161200
F	4.49596000	1.54789800	-2.35964800
F	-1.98892400	0.55890900	-4.63178300
F	-2.30317700	-1.96780000	-4.17949400
F	0.15897800	-1.81270500	-4.85164400
F	0.85372700	-3.85194900	-3.74403000
F	2.99413100	-3.62611600	-2.46582500
F	3.66461700	-1.39601100	-3.59690100
F	-2.74217100	4.45687400	0.98348000
F	-0.40928400	5.06583300	0.91032200
F	2.68388700	0.03060200	4.61075500
F	0.64718700	-1.24009800	5.24351200
F	0.42962500	-3.32001200	3.99695800
F	-2.11458600	-3.11984700	3.59749200
F	-4.30948200	-1.53560200	2.21334600
F	-4.75473700	0.82763600	1.43394700
F	-3.50817600	1.40349600	3.51454400
F	-2.21095000	3.41389200	3.14573400
F	-0.87835800	0.69424000	5.02089100
O	-4.18683100	2.94591700	-0.30241500
H	-4.19701200	3.91575200	-0.37596200
H	-5.70205600	0.68185500	-0.29016700
IP			
C	-2.63229800	-1.09834200	-1.19878300
C	-2.75538800	0.31546400	-1.30752600
C	-2.52201400	1.04361300	-2.59139100
C	-2.22418300	2.55408500	-2.06313000
C	-0.72287800	3.01894400	-2.23776200
C	0.03256900	3.87158200	-1.11549700
C	1.60676800	3.35297000	-1.21351600
C	2.45290000	3.08403300	0.06971300
C	3.64028800	1.92368200	0.08388700
C	3.45455800	1.21891200	1.51447900
C	3.73985400	-0.31897700	1.71344400
C	2.66471400	-1.09309700	2.70502900
C	1.87893400	-1.88931600	1.72750400

C	0.61572400	-2.40231400	1.93344500
C	-0.06559900	-2.99824000	0.88814100
C	-1.46857400	-3.34335000	1.23261900
C	-2.41952300	-3.19812300	-0.02713300
C	-3.26373800	-1.85737700	-0.07772300
C	-1.90712400	-1.84491100	-2.03336900
C	-1.68039500	-3.23382300	-1.51843900
C	-0.14880800	-3.56980600	-1.58786000
C	0.52104100	-3.09741200	-0.35153500
C	1.78791900	-2.58826600	-0.55822500
C	2.45218500	-1.95656900	0.47356200
C	3.74506400	-1.22654700	0.38774000
C	3.95243100	-0.59962700	-1.03985600
C	3.64812100	0.97141700	-1.17325200
C	2.34014900	0.99973800	-1.87829600
C	1.44156900	2.04698400	-1.89956000
C	0.18821200	1.86247000	-2.44327700
C	-0.13374100	0.65964500	-3.02835100
C	-1.49143900	0.26827200	-3.46977100
C	-1.38935700	-1.33931100	-3.34494000
C	0.15974400	-1.66225400	-3.50238900
C	0.77268800	-2.91205000	-2.75055200
C	2.21596600	-2.60745700	-1.97953200
C	3.01590600	-1.28204600	-2.23189700
C	2.01529400	-0.20906500	-2.46369600
C	0.77000200	-0.38623600	-3.02855200
C	-3.01526400	1.09060000	-0.25600600
C	-2.87642000	2.55538400	-0.57834400
C	-2.11343300	3.34098000	0.56242000
C	-0.58967200	3.79927700	0.32199100
C	0.17934900	2.88781500	1.20919200
C	1.52184800	2.57069400	1.10738200
C	2.05798000	1.57067600	1.89206600
C	1.27508600	0.94306700	2.84286300
C	1.64622000	-0.29443100	3.58403100
C	0.15622300	-0.93674000	3.93668200
C	-0.22680300	-2.25475800	3.15161600
C	-1.68409100	-2.43480500	2.52699500
C	-2.28475800	-1.11515600	2.16680200
C	-3.43607900	-1.01168900	1.21428800
C	-3.59137600	0.56106700	1.02443600
C	-2.88266700	1.20026100	2.26166600
C	-2.07198400	2.55499500	1.98647600
C	-0.61230600	2.25904900	2.14478300

C	-0.05322200	1.29589600	2.97291400
C	-0.85763100	0.27589500	3.70590500
C	-1.99863400	0.04403200	2.75917700
F	-3.71110700	1.08045400	-3.28411400
F	-2.97256500	3.42139300	-2.80527300
F	-0.68682900	3.78356000	-3.38930500
F	-0.00065900	5.17334600	-1.50223000
F	2.27393500	4.25435400	-2.00408800
F	3.04112200	4.25767100	0.46921300
F	4.83871800	2.56105300	0.10384000
F	4.30131200	1.87924700	2.38261500
F	4.97095500	-0.42278200	2.27614200
F	3.39961800	-1.90930500	3.52853200
F	-1.53372100	-4.65831600	1.63695100
F	-3.28686100	-4.24204300	0.01167900
F	-4.53708400	-2.18037700	-0.50815000
F	-2.34056100	-4.16110300	-2.28271100
F	-0.02468900	-4.93610900	-1.69684500
F	4.76231200	-2.14570900	0.55458300
F	5.25362300	-0.78928700	-1.37547800
F	4.60538500	1.47753000	-2.03003300
F	-1.70802100	0.57905500	-4.79029700
F	-2.08985700	-1.94128700	-4.35557600
F	0.41952000	-1.82767200	-4.84470100
F	0.99940500	-3.87098200	-3.68137000
F	3.03822000	-3.67350400	-2.24352400
F	3.82768300	-1.45811000	-3.32323300
F	-2.81858300	4.50528700	0.75229700
F	-0.47906600	5.07340200	0.84896400
F	2.24248200	0.00536600	4.78291200
F	0.14491400	-1.23505200	5.26070600
F	-0.00832500	-3.31415400	4.00320600
F	-2.51007900	-3.07588900	3.41152100
F	-4.56378800	-1.47838300	1.85665300
F	-4.92401100	0.88500900	1.04591300
F	-3.82704100	1.47084400	3.21714800
F	-2.47018500	3.45655100	2.94364900
F	-1.32750800	0.72388500	4.92109000
O	-4.18804000	3.03781100	-0.65464300
H	-4.16308000	4.00961000	-0.68553000
C ₁ -S _N 2'-C41-F _e			
RC			
C	-2.75992600	-1.15693200	-1.00372300
C	-3.37611000	0.19583500	-1.09934500

C	-2.86694100	1.12161700	-2.26495600
C	-2.38515800	2.47548100	-1.48565300
C	-1.02599100	3.12125900	-1.88163700
C	-0.18246500	3.94119800	-0.77506300
C	1.38977000	3.51874500	-1.09399400
C	2.39825400	3.21223400	0.06022300
C	3.62724000	2.11638600	-0.15407500
C	3.64910000	1.30330900	1.22891700
C	4.02392300	-0.22846400	1.27031500
C	3.11168500	-1.13120300	2.31285300
C	2.25629500	-1.90030300	1.37253700
C	1.05091000	-2.49497700	1.68042500
C	0.28013700	-3.04831000	0.67553500
C	-1.05922900	-3.48823100	1.14508800
C	-2.15506800	-3.29728300	0.01277000
C	-3.12030500	-2.03507800	0.16529200
C	-1.95825900	-1.73818600	-1.88958500
C	-1.58335600	-3.14622500	-1.52272700
C	-0.07496500	-3.42754900	-1.80502500
C	0.72341800	-3.02500900	-0.62465800
C	1.93265700	-2.43724900	-0.93588600
C	2.68202200	-1.84517600	0.06018600
C	3.91701400	-1.03610500	-0.11506400
C	3.92127600	-0.29797500	-1.50364600
C	3.52996000	1.25878800	-1.47561800
C	2.14831800	1.26497100	-2.02196200
C	1.21025100	2.26343800	-1.86674500
C	-0.08502200	2.05471700	-2.29024700
C	-0.43670000	0.86839900	-2.89038300
C	-1.81571100	0.42902100	-3.22723500
C	-1.62295000	-1.15516000	-3.22422300
C	-0.08997300	-1.38703600	-3.58294100
C	0.66881600	-2.65031400	-3.01188300
C	2.18224000	-2.32506100	-2.39539000
C	2.88073000	-0.94198200	-2.63090400
C	1.80846300	0.08586900	-2.65726800
C	0.51122200	-0.12011900	-3.07923700
C	-3.02615200	0.90198300	0.17347900
C	-2.42373000	2.07193100	-0.03450600
C	-2.03134700	3.03477000	1.03624300
C	-0.63471500	3.73402600	0.72607500
C	0.30685200	2.85449100	1.48000800
C	1.63192100	2.59626600	1.17669300
C	2.29877100	1.56014000	1.80325700

C	1.66384800	0.81850700	2.78174400
C	2.16918000	-0.45689200	3.36273600
C	0.75895900	-1.20294700	3.82601200
C	0.34799300	-2.48038500	2.99153200
C	-1.16205700	-2.69381300	2.51808600
C	-1.85996400	-1.38905400	2.32112700
C	-3.13689500	-1.28908900	1.53869800
C	-3.39410900	0.27924800	1.48959500
C	-2.54350500	0.87392000	2.67081300
C	-1.83141600	2.28368400	2.42048000
C	-0.34181400	2.09928300	2.44181600
C	0.34672400	1.09175500	3.09801600
C	-0.32976000	-0.03665700	3.80272000
C	-1.55318200	-0.26044300	2.95913800
F	-4.74871600	0.02327300	-1.20946400
F	-3.94610900	1.45746100	-3.02622100
F	-3.34907300	3.43960900	-1.69783400
F	-1.25823700	3.97113800	-2.94036800
F	-0.31606000	5.26066700	-1.05716500
F	1.91540100	4.51282700	-1.88150900
F	2.98166700	4.38991500	0.45501900
F	4.78962300	2.81431500	-0.22617500
F	4.57078900	1.94130800	2.03590300
F	5.31610200	-0.30681500	1.67949900
F	3.97664200	-1.96232700	2.98079800
F	-1.02101100	-4.83190500	1.44480300
F	-2.93555100	-4.40907000	0.03992300
F	-4.40831100	-2.47551200	-0.05586900
F	-2.30947400	-4.00577900	-2.31340800
F	0.06431500	-4.77744600	-2.03524400
F	4.99141400	-1.90325600	-0.13877400
F	5.17942900	-0.39081400	-2.00304900
F	4.35285400	1.87903300	-2.39463400
F	-2.13093000	0.80421000	-4.51338100
F	-2.41474700	-1.74074300	-4.17561000
F	0.01285600	-1.43498700	-4.95515100
F	0.82196700	-3.52684400	-4.03425200
F	3.01265400	-3.32039000	-2.84344100
F	3.56301300	-0.98875900	-3.81966500
F	-3.00093100	3.99177300	1.14427100
F	-0.66263900	4.97871300	1.31520600
F	2.88815500	-0.22428000	4.50838000
F	0.91369600	-1.59347500	5.11665100
F	0.70917600	-3.58503600	3.72931300

F	-1.85266500	-3.43795400	3.43733700
F	-4.13535200	-1.86493200	2.29466700
F	-4.72641400	0.51129600	1.71201400
F	-3.36596200	1.01646600	3.75803300
F	-2.23191700	3.13543000	3.41857900
F	-0.70133800	0.27580300	5.09254400
H	-5.52150300	2.96408100	-0.98775300
O	-5.57763900	2.59718000	-0.09318100
H	-6.12330700	1.80385300	-0.19530000
TS	imaginary vibrational frequency		-801.06 cm ⁻¹
C	-2.76425500	-1.27162900	-0.96807600
C	-3.26210600	0.10933900	-1.10400800
C	-2.86747900	0.92510600	-2.36209200
C	-2.48803800	2.41825200	-1.73744900
C	-1.05132600	2.96464500	-2.08706700
C	-0.21293600	3.86388800	-1.05727100
C	1.36246100	3.42166600	-1.33432600
C	2.36572800	3.20187100	-0.15595700
C	3.60145300	2.09904800	-0.28153300
C	3.61444900	1.38614300	1.15762500
C	3.99226000	-0.13771000	1.31411000
C	3.07182600	-0.96590400	2.41233700
C	2.22218700	-1.79809700	1.52247100
C	1.01293100	-2.36826900	1.86161400
C	0.25186900	-2.99315600	0.89261900
C	-1.08776900	-3.40760200	1.38172200
C	-2.17218700	-3.30996700	0.22884400
C	-3.13265900	-2.03810200	0.27149300
C	-1.97407100	-1.92773600	-1.80801800
C	-1.59004800	-3.29274100	-1.31866500
C	-0.07171300	-3.56849500	-1.55737800
C	0.70781500	-3.06723900	-0.40170300
C	1.91970600	-2.50244800	-0.74324900
C	2.65961900	-1.83788700	0.21349600
C	3.89614000	-1.04277000	-0.00988900
C	3.91039000	-0.40517400	-1.44785300
C	3.51256900	1.14817300	-1.53614700
C	2.13082900	1.10762700	-2.08127700
C	1.18236000	2.10538500	-1.99312000
C	-0.11574400	1.85293600	-2.38300100
C	-0.44538000	0.63161700	-2.91728700
C	-1.81009900	0.17648500	-3.26078200
C	-1.61966900	-1.41561500	-3.16572900
C	-0.07732300	-1.65736400	-3.47769900

C	0.67889600	-2.87494600	-2.81070300
C	2.18512600	-2.49836700	-2.20441800
C	2.88025500	-1.13247700	-2.53193000
C	1.80225900	-0.11569400	-2.63144300
C	0.50897800	-0.35902000	-3.04134300
C	-2.74240600	0.85322200	0.06648000
C	-2.80298700	2.27831300	-0.20975100
C	-2.11630100	3.20296400	0.83411300
C	-0.66037000	3.76182700	0.44065700
C	0.25648800	2.90782300	1.24289700
C	1.59015700	2.65208100	0.98589100
C	2.25627200	1.67308500	1.69685800
C	1.61368900	1.00210100	2.72107600
C	2.12055200	-0.22103700	3.40434200
C	0.70963300	-0.93625100	3.91381200
C	0.30228700	-2.26805900	3.16536000
C	-1.20859700	-2.52429400	2.70278300
C	-1.91330600	-1.23831700	2.42784900
C	-3.15472900	-1.14927800	1.56475300
C	-3.16491400	0.38365300	1.31448700
C	-2.56903100	1.05354800	2.55202300
C	-1.87370400	2.44249500	2.24501900
C	-0.39387200	2.23562200	2.25534700
C	0.29218600	1.28935200	3.00208500
C	-0.37898200	0.22424400	3.80619000
C	-1.60351000	-0.06795400	2.99119000
F	-4.68082900	0.05325900	-1.09650400
F	-3.97527800	1.11852300	-3.13736600
F	-3.38631800	3.31263500	-2.28007700
F	-1.20650900	3.71692400	-3.23514500
F	-0.35576000	5.15872800	-1.43839000
F	1.88918400	4.34885300	-2.19790200
F	2.93938200	4.40603600	0.16639200
F	4.76182900	2.79447400	-0.39554900
F	4.52618000	2.08473200	1.92459200
F	5.28125600	-0.18269400	1.73805000
F	3.93312800	-1.74659700	3.14314900
F	-1.03874900	-4.72707400	1.77663500
F	-2.95561100	-4.41462500	0.34521300
F	-4.42013200	-2.49501200	0.09228400
F	-2.28803100	-4.24304100	-2.02640900
F	0.09811800	-4.92947800	-1.68224000
F	4.97167200	-1.90802700	0.03575700
F	5.17342900	-0.52756200	-1.92862800

F	4.33562300	1.70287700	-2.49620200
F	-2.09330200	0.48151000	-4.57400500
F	-2.38403500	-2.04727300	-4.11013200
F	0.06175600	-1.79096900	-4.84161100
F	0.84615100	-3.82108000	-3.76710800
F	3.02524600	-3.51929500	-2.56961600
F	3.56862800	-1.25675500	-3.71177000
F	-2.89824600	4.29360600	1.05864000
F	-0.59542500	5.04297100	0.95214000
F	2.83013400	0.10159200	4.53397200
F	0.86027700	-1.23838800	5.22856600
F	0.66657100	-3.31842400	3.97755000
F	-1.89330100	-3.21957500	3.66437600
F	-4.23478200	-1.53603900	2.32269700
F	-4.83158700	0.90266700	1.43713200
F	-3.49591200	1.24433500	3.54171100
F	-2.24040800	3.31753200	3.23845300
F	-0.73476900	0.64562000	5.06980300
H	-4.74920600	1.83467200	0.63889300
O	-4.34192700	2.67006700	-0.04518000
H	-4.76672500	2.68661000	-0.92580400
PC			
C	-2.67951500	-1.57441000	-0.56046700
C	-3.48671400	-0.32509700	-0.44639500
C	-3.36142800	0.70288600	-1.62183500
C	-3.08219100	2.17526200	-0.88698500
C	-1.80141700	2.95196300	-1.38844000
C	-0.90993900	3.84917300	-0.40659800
C	0.62867800	3.69813900	-1.01724400
C	1.86567500	3.50712700	-0.08082300
C	3.19168900	2.63884300	-0.57893300
C	3.58504000	1.77991700	0.72009300
C	4.19215400	0.33007900	0.59002300
C	3.63099200	-0.75264600	1.71042000
C	2.74071800	-1.60398100	0.87986300
C	1.71091500	-2.39261000	1.34981200
C	0.86162500	-3.01602100	0.45613900
C	-0.28403100	-3.69303700	1.11441700
C	-1.57978100	-3.62914100	0.19703500
C	-2.67004500	-2.54161600	0.59423500
C	-1.97930300	-1.99157200	-1.60876200
C	-1.32809700	-3.33139200	-1.40130700
C	0.13114700	-3.35099500	-1.95044900
C	1.05510700	-2.87043400	-0.89710200

C	2.08850700	-2.08857700	-1.37070000
C	2.90921700	-1.42729200	-0.47941200
C	3.95740000	-0.42499400	-0.80884200
C	3.59810700	0.36275900	-2.12261200
C	2.98444000	1.83262500	-1.91808100
C	1.54001100	1.63204500	-2.20402100
C	0.50280800	2.44753900	-1.80462100
C	-0.80056900	2.03432600	-1.97950500
C	-1.06268900	0.84811700	-2.61490600
C	-2.39532700	0.22832500	-2.77892300
C	-1.97849900	-1.30573900	-2.93432700
C	-0.51208900	-1.27103800	-3.55581200
C	0.51902800	-2.41896500	-3.21114900
C	2.05348900	-1.87996500	-2.84100700
C	2.47996200	-0.39371400	-3.09502800
C	1.27638600	0.44228900	-2.85452300
C	-0.02801900	0.04477600	-3.05462600
C	-3.06631400	0.38923100	0.80213100
C	-3.22756800	1.88987900	0.69072200
C	-2.30506600	2.70627200	1.69988000
C	-1.03249200	3.50321400	1.11381700
C	0.12640800	2.70424300	1.59753700
C	1.40938700	2.70535900	1.08347300
C	2.33113800	1.77652100	1.52285700
C	2.00207900	0.90121200	2.54213800
C	2.80240400	-0.28602800	2.95222700
C	1.63494900	-1.27210800	3.60818400
C	1.27402400	-2.56020700	2.76320900
C	-0.24869400	-3.00833500	2.55723800
C	-1.16102700	-1.83256700	2.60911200
C	-2.52905800	-1.81162500	1.96085000
C	-2.72798000	-0.30403700	1.88553500
C	-2.09852000	0.30915700	3.10220700
C	-1.67439600	1.80674000	2.90145100
C	-0.21123900	1.82987600	2.60612000
C	0.73453600	0.93613600	3.08880500
C	0.39698500	-0.29487200	3.86812700
C	-0.92021400	-0.69468100	3.27109800
F	-4.83189600	-0.69694000	-0.34250100
F	-4.60608000	0.80722800	-2.21733800
F	-4.14498800	2.95957400	-1.23661700
F	-2.23264100	3.79468300	-2.39653200
F	-1.29569500	5.13956300	-0.56779500
F	0.84619000	4.78312500	-1.82745700

F	2.32344600	4.73996700	0.30942400
F	4.20170000	3.51797800	-0.79996700
F	4.52289300	2.52579600	1.40602900
F	5.53354600	0.44560400	0.76252400
F	4.71832900	-1.46266500	2.15517700
F	0.01472700	-5.02619800	1.28977000
F	-2.17227600	-4.84895500	0.28571300
F	-3.89553600	-3.17106800	0.59763500
F	-2.04015400	-4.27156700	-2.10857300
F	0.43451400	-4.65032400	-2.28957500
F	5.12724300	-1.10695500	-1.07940200
F	4.74393500	0.49760300	-2.83663100
F	3.51490600	2.61564800	-2.92370300
F	-2.95597900	0.62706400	-3.97236600
F	-2.83050900	-1.95781300	-3.78398400
F	-0.64022500	-1.23366100	-4.92564800
F	0.61570400	-3.21763300	-4.30175700
F	2.93048600	-2.70851100	-3.49258900
F	2.92963000	-0.27579200	-4.38479100
F	-3.08415600	3.65103500	2.28243200
F	-0.99191100	4.71378600	1.77893800
F	3.67147600	0.02554800	3.96716500
F	2.08890700	-1.69237300	4.81579200
F	1.94124000	-3.62094800	3.33342900
F	-0.61529400	-3.92055900	3.51056600
F	-3.43437500	-2.38083400	2.84097700
F	-6.56399400	1.40591200	-0.48898500
F	-2.93625600	0.22386300	4.19214600
F	-1.92437100	2.46509800	4.08088700
F	0.26954800	-0.05962600	5.21938100
H	-6.12501800	1.00243000	-1.21874000
O	-4.52310300	2.21156500	1.10824400
H	-5.21558700	1.87720200	0.49486900
IP			
C	-3.02359500	-0.94612400	-0.68444900
C	-3.52798900	0.45674100	-0.65012200
C	-3.13943500	1.38729900	-1.85088900
C	-2.56737700	2.78873000	-1.14216000
C	-1.13000200	3.25346600	-1.59327300
C	-0.11669400	3.97555000	-0.58720500
C	1.37987000	3.47133100	-1.10401900
C	2.49627600	3.05652700	-0.09288400
C	3.62429400	1.90324900	-0.48842600
C	3.75579800	1.03368800	0.85526900

C	4.04064100	-0.51631400	0.80297900
C	3.20461500	-1.40625700	1.92183300
C	2.19307400	-2.08139400	1.06811900
C	0.99472000	-2.61033100	1.50165000
C	0.07403100	-3.06969100	0.57961100
C	-1.22249700	-3.45729000	1.18997000
C	-2.42746100	-3.15372500	0.19794500
C	-3.27460500	-1.84275900	0.50061700
C	-2.37766600	-1.54597800	-1.67787100
C	-2.03959000	-2.98369700	-1.39233900
C	-0.59273000	-3.33701800	-1.85429000
C	0.35961500	-3.02251600	-0.76419700
C	1.55979100	-2.50126300	-1.20084800
C	2.46137700	-1.99939600	-0.28412300
C	3.71695400	-1.26100800	-0.58366200
C	3.60212000	-0.46863400	-1.93870300
C	3.31402300	1.10576000	-1.81281600
C	1.87697300	1.21033100	-2.17565800
C	1.02439100	2.24717900	-1.86245800
C	-0.32700600	2.11901800	-2.10252900
C	-0.81257600	0.99173500	-2.71491700
C	-2.24050100	0.66721200	-2.93385600
C	-2.15862900	-0.92754600	-3.01953900
C	-0.68951200	-1.23513600	-3.55421600
C	0.04990100	-2.56287200	-3.11752300
C	1.64368500	-2.35235000	-2.67643100
C	2.39528000	-1.00545800	-2.94995100
C	1.39187300	0.07969400	-2.80347100
C	0.04347600	-0.03427100	-3.06692000
C	-3.00267100	1.10206000	0.59396300
C	-2.83656000	2.59030600	0.42679300
C	-1.83551600	3.24220100	1.46548200
C	-0.39174000	3.72709300	0.93361900
C	0.54200900	2.71924000	1.50725100
C	1.81785500	2.42135100	1.06632400
C	2.49221500	1.33347500	1.58365700
C	1.93235700	0.59260100	2.60851100
C	2.43585400	-0.72051300	3.09920900
C	1.05238200	-1.40475500	3.71697500
C	0.46274100	-2.62058700	2.89224500
C	-1.10930800	-2.73943000	2.61341200
C	-1.74615800	-1.39402600	2.58137800
C	-3.04101600	-1.10412100	1.85140400
C	-2.89474000	0.40404900	1.71946500

C	-2.21775400	0.91925300	2.95419900
C	-1.47233700	2.28235000	2.73153400
C	-0.02611300	1.97889200	2.51988600
C	0.67770900	0.92242300	3.08175600
C	0.04530500	-0.17453200	3.87834300
C	-1.29678400	-0.30784600	3.22234700
F	-4.92472000	0.42479400	-0.57167500
F	-4.29512400	1.74287300	-2.48282100
F	-3.41344200	3.77663100	-1.55714000
F	-1.31953700	4.13078000	-2.64488000
F	-0.20348700	5.31181900	-0.80574400
F	1.86869100	4.45158800	-1.92955600
F	3.19146400	4.17617700	0.28787400
F	4.81118500	2.53422800	-0.67624900
F	4.79664600	1.58794100	1.57384600
F	5.36545200	-0.68327800	1.04752300
F	4.08981500	-2.31261500	2.45025800
F	-1.22976900	-4.81540700	1.42057000
F	-3.27361800	-4.21331500	0.28969100
F	-4.60620500	-2.19445800	0.46116300
F	-2.89918600	-3.78195400	-2.10977400
F	-0.55901600	-4.68446700	-2.13540600
F	4.72272100	-2.18916700	-0.76680600
F	4.78348900	-0.61448300	-2.59003300
F	4.05299800	1.71326000	-2.80831200
F	-2.64286900	1.12523800	-4.16843900
F	-3.08504100	-1.41681900	-3.89992700
F	-0.73604600	-1.22881000	-4.92992600
F	0.02422200	-3.40830000	-4.17642100
F	2.35099000	-3.37855800	-3.24891400
F	2.92330600	-1.04123400	-4.21475400
F	-2.43781800	4.35160700	1.96454600
F	-0.13314900	4.92742800	1.56729000
F	3.30014500	-0.55948500	4.15257000
F	1.34509100	-1.86199000	4.96060900
F	0.85526600	-3.77385400	3.53316000
F	-1.71061200	-3.51298500	3.57020600
F	-4.09346100	-1.41785100	2.69559200
F	-3.11295600	1.06307600	3.99124100
F	-1.63505600	3.03270000	3.87034200
F	-0.09173400	0.13913400	5.21278700
O	-4.08500700	3.17635500	0.74295300
H	-4.76349300	2.81117800	0.14795900

C₁- S_N2'-C1-F_j

RC

C	-3.10729200	-0.45472700	-0.39845000
C	-3.37623700	1.00749600	-0.50907500
C	-2.88759400	1.71560900	-1.82616100
C	-1.96732100	2.95293600	-1.26349400
C	-0.59381300	3.23272500	-1.93441200
C	0.60248200	3.87749200	-1.05838800
C	1.94947500	3.06953800	-1.58601000
C	3.05277600	2.58981600	-0.58617800
C	3.93895000	1.21932300	-0.89168700
C	4.02240300	0.49872600	0.53989700
C	4.03552800	-1.07404900	0.66449000
C	3.14253600	-1.67276500	1.92129400
C	1.97824400	-2.25879200	1.20848700
C	0.74340200	-2.52730800	1.76109300
C	-0.30247600	-2.92605400	0.95020700
C	-1.60125300	-3.00514700	1.66763800
C	-2.81171900	-2.61562200	0.71443600
C	-3.42495300	-1.15174100	0.89990800
C	-2.62630400	-1.26065900	-1.34072000
C	-2.50881400	-2.69296200	-0.90117200
C	-1.17306000	-3.33993900	-1.39292400
C	-0.10576900	-3.07931000	-0.40047900
C	1.13094700	-2.82125400	-0.95580300
C	2.16261800	-2.37714300	-0.15455300
C	3.49848500	-1.90289400	-0.60311600
C	3.42310800	-1.26081900	-2.03701700
C	3.41096900	0.34344400	-2.09266000
C	1.99215500	0.65563100	-2.40449700
C	1.34929000	1.85764000	-2.19856900
C	-0.01430800	1.94835000	-2.38954200
C	-0.73259300	0.85042500	-2.80663800
C	-2.21636600	0.73335700	-2.87524200
C	-2.38845000	-0.85264600	-2.76035600
C	-1.02835700	-1.45667700	-3.32302100
C	-0.49516900	-2.83364600	-2.77039300
C	1.13602400	-2.85221700	-2.43986900
C	2.07712900	-1.69236300	-2.91331700
C	1.28274100	-0.43838700	-2.85888600
C	-0.08062400	-0.34589000	-3.04226300
C	-2.61991700	1.65428000	0.61146700
C	-1.82707000	2.64297600	0.20346100
C	-1.04342300	3.53727400	1.10474300
C	0.39387300	3.86605300	0.51032100

C	1.22889600	2.82705300	1.18344500
C	2.38190900	2.23940500	0.69479300
C	2.89388300	1.10633600	1.29941500
C	2.29243900	0.59241900	2.43325800
C	2.58494700	-0.73630200	3.04167400
C	1.14718700	-1.09317100	3.79421800
C	0.30936900	-2.27484600	3.16107400
C	-1.27023100	-2.14081900	2.96025300
C	-1.67284400	-0.71890200	2.75636700
C	-3.01130400	-0.34983100	2.18182000
C	-2.89085000	1.22286200	2.02226900
C	-1.73705800	1.65552100	2.99461400
C	-0.77874000	2.83698000	2.50413000
C	0.60833100	2.30157700	2.30412800
C	1.15167100	1.19214900	2.93143300
C	0.37026500	0.29884100	3.83683500
C	-1.00181100	0.33243200	3.22557600
F	-4.72492600	1.24865300	-0.31032800
F	-3.96595700	2.28463000	-2.43304600
F	-2.71425200	4.10379600	-1.37690100
F	-0.81323800	4.06227600	-3.01128200
F	0.72966400	5.17392900	-1.43523200
F	2.54016700	3.86311300	-2.53813100
F	3.95141400	3.61161500	-0.40691100
F	5.19793600	1.61088600	-1.21589000
F	5.19597600	0.93562500	1.12267600
F	5.32705600	-1.44208700	0.86402900
F	3.89936400	-2.65211800	2.51558100
F	-1.81630400	-4.30108100	2.08154300
F	-3.80504300	-3.50438200	0.97629300
F	-4.79414300	-1.28292400	0.95391300
F	-3.53292300	-3.40815000	-1.47345300
F	-1.38434900	-4.69509300	-1.51273200
F	4.32178600	-3.00541500	-0.71987300
F	4.51607200	-1.68158100	-2.72241100
F	4.17410100	0.69703800	-3.18788300
F	-2.66536500	1.10543600	-4.12412900
F	-3.40499500	-1.30788400	-3.55542800
F	-1.17152300	-1.59596300	-4.68693200
F	-0.73358600	-3.77356100	-3.71764600
F	1.62520200	-4.04039800	-2.91973400
F	2.50397300	-1.96197400	-4.18860600
F	-1.74372900	4.70225100	1.27897200
F	0.75306600	5.11135400	0.97665300

F	3.53077100	-0.62585000	4.02994300
F	1.43621100	-1.44093800	5.07400600
F	0.53366100	-3.39320500	3.93172900
F	-1.93559700	-2.64529400	4.04553100
F	-3.96270100	-0.61165500	3.14392800
F	-4.06863900	1.81098700	2.41000800
F	-2.30400200	2.05240300	4.17859000
F	-0.79425600	3.81468500	3.46728700
F	0.31449900	0.76036700	5.13453600
H	-5.94968600	0.76503200	-2.32525300
O	-5.56416100	-0.09912300	-2.52866200
H	-5.45343400	-0.09813300	-3.49056000
TS	imaginary vibrational frequency		-741.72 cm ⁻¹
C	-3.43759000	-0.23025200	-0.82710700
C	-3.35233900	1.29556700	-0.76147300
C	-2.61004800	2.04145500	-1.96506700
C	-1.68543000	3.15326800	-1.21521700
C	-0.23487500	3.42165700	-1.73364600
C	0.90491400	3.91818200	-0.69719200
C	2.26202400	3.08192300	-1.16770000
C	3.23268200	2.45004700	-0.11609200
C	4.06800100	1.05474100	-0.45666700
C	3.97377500	0.21735800	0.90864200
C	3.88783800	-1.35906300	0.89970100
C	2.85555300	-2.00072900	2.01869500
C	1.73745200	-2.47596100	1.16286100
C	0.44807100	-2.72883200	1.58461600
C	-0.53572500	-3.02320900	0.65851300
C	-1.90107900	-3.02213700	1.25367100
C	-2.97503200	-2.45575900	0.21337500
C	-3.66682800	-1.02720900	0.51088200
C	-2.32900500	-0.87070600	-1.51236500
C	-2.38759600	-2.24205600	-1.24134600
C	-1.24261200	-3.10080800	-1.78451400
C	-0.22934200	-3.08340600	-0.68374500
C	1.06146500	-2.82818900	-1.10693400
C	2.03621000	-2.49772900	-0.18461400
C	3.42758300	-2.05372800	-0.47357000
C	3.52152700	-1.29373000	-1.84657800
C	3.61271900	0.31011100	-1.77057200
C	2.25685800	0.74461000	-2.19460300
C	1.66969300	1.96824600	-1.94906600
C	0.33841100	2.16214600	-2.25963100
C	-0.38706100	1.15105800	-2.83301100

C	-1.86077000	1.10941600	-2.99663100
C	-2.09101900	-0.43796500	-2.91493400
C	-0.79758400	-1.09331200	-3.51549700
C	-0.39305000	-2.53913700	-3.04027800
C	1.19399100	-2.70001200	-2.58019700
C	2.24482600	-1.56775500	-2.86985300
C	1.53367800	-0.26552800	-2.80399700
C	0.20835000	-0.06693000	-3.11462600
C	-2.57248800	1.71721400	0.45712800
C	-1.69455800	2.69070500	0.21378400
C	-0.96056700	3.47560000	1.25534800
C	0.54053600	3.78458100	0.83399900
C	1.26133400	2.65493300	1.49267100
C	2.42255000	2.03917800	1.06157700
C	2.81424600	0.83274200	1.61193300
C	2.08377600	0.26902600	2.64034800
C	2.24690800	-1.11923900	3.15651900
C	0.73259200	-1.44578500	3.74670400
C	-0.10337000	-2.52657400	2.95297200
C	-1.64070900	-2.26909400	2.61645800
C	-1.94339300	-0.81774300	2.47467000
C	-3.21747700	-0.31786500	1.84988100
C	-2.99127700	1.23343000	1.80833200
C	-1.91718000	1.52315500	2.91565200
C	-0.86113800	2.67621200	2.61681500
C	0.51251700	2.08229400	2.50667800
C	0.93658500	0.89708800	3.08524300
C	0.02622900	-0.01778000	3.83374700
C	-1.27307400	0.14866400	3.09879700
F	-4.63126700	1.80967600	-0.65905100
F	-3.57227400	2.70702600	-2.66577000
F	-2.36196800	4.35081600	-1.27484800
F	-0.32248300	4.36227300	-2.73488700
F	1.13189200	5.23224100	-0.94226600
F	2.98387400	3.92616600	-1.97459800
F	4.16541000	3.39287600	0.23810100
F	5.37171100	1.39315000	-0.62812700
F	5.10840700	0.53087600	1.63162100
F	5.13502800	-1.81862600	1.17918800
F	3.50792200	-3.06005900	2.60099500
F	-2.27100500	-4.31096000	1.56176800
F	-3.97783500	-3.37449000	0.20950300
F	-5.00408700	-1.25846900	0.66002400
F	-3.81378900	-2.77022700	-2.13869200

F	-1.66406600	-4.37333500	-2.06865100
F	4.20621800	-3.18679900	-0.60918000
F	4.64783500	-1.73003500	-2.46657400
F	4.50658700	0.68919500	-2.75298900
F	-2.20176600	1.54591200	-4.26041200
F	-3.18944100	-0.73528000	-3.74894800
F	-0.91185100	-1.12266900	-4.88828100
F	-0.60118300	-3.38496500	-4.07984700
F	1.65182500	-3.86670100	-3.14131500
F	2.77560000	-1.78107500	-4.11740800
F	-1.63385000	4.65502700	1.44344400
F	0.89394600	4.96826700	1.44376200
F	3.10340000	-1.14221900	4.22936600
F	0.88397000	-1.90262300	5.01627200
F	-0.03188300	-3.70272600	3.66542200
F	-2.44042800	-2.79210700	3.59968000
F	-4.21931300	-0.56318500	2.76793600
F	-4.16619400	1.87427700	2.12028300
F	-2.58012000	1.85617300	4.06934200
F	-0.92667700	3.58622800	3.64205800
F	-0.13673100	0.34102600	5.15460100
H	-4.48984200	-1.69138400	-1.93316100
O	-4.76199100	-0.62715000	-1.65393900
H	-4.71700800	-0.15157400	-2.50995000
PC			
C	3.68259200	0.53420100	-0.41102000
C	3.40652700	-0.84596800	-1.06479900
C	2.79059900	-0.86968900	-2.52854600
C	1.81972300	-2.18825300	-2.49122000
C	0.41538000	-2.12660000	-3.16224200
C	-0.78603500	-3.05083600	-2.59106300
C	-2.11433200	-2.05989300	-2.66619400
C	-3.17131200	-2.02226000	-1.51182700
C	-4.00334400	-0.62588400	-1.16495200
C	-4.01968900	-0.58427600	0.43867600
C	-3.96403300	0.78423500	1.22522800
C	-3.02125700	0.76724200	2.58393700
C	-1.86394100	1.60415600	2.16806700
C	-0.60890300	1.59761800	2.75098300
C	0.42574100	2.30733300	2.16874400
C	1.77000600	1.94967900	2.72750300
C	2.86248400	1.92189200	1.55092600
C	3.63236400	0.55794200	1.20767600
C	2.68743000	1.58836000	-0.81456000

C	2.28136300	2.34889700	0.19810100
C	1.27634000	3.46502500	0.09827600
C	0.19060200	3.02774600	1.01353700
C	-1.05846300	3.03698400	0.42696100
C	-2.08071600	2.30057900	0.99456100
C	-3.43275400	2.06618300	0.41706100
C	-3.40635900	2.08865700	-1.15777700
C	-3.46295200	0.66271600	-1.89240000
C	-2.06574500	0.47114600	-2.35839400
C	-1.47785900	-0.72092800	-2.72334700
C	-0.12688300	-0.75973000	-2.99608500
C	0.62842200	0.38602200	-2.92382800
C	2.10729300	0.47238200	-3.01841200
C	2.38283000	1.84383800	-2.25954900
C	1.03053900	2.68718000	-2.42873300
C	0.54985500	3.68575400	-1.30359800
C	-1.07464000	3.63764500	-0.93454800
C	-2.06505500	2.80757300	-1.81360200
C	-1.31749800	1.63132700	-2.32544500
C	0.03517100	1.58997000	-2.59614400
C	2.53963400	-1.76907000	-0.26716600
C	1.71015400	-2.48885600	-1.02208000
C	0.92943800	-3.67683900	-0.55788900
C	-0.53291900	-3.70727700	-1.17546800
C	-1.31450200	-3.04165100	-0.08994300
C	-2.45418800	-2.27108000	-0.23273100
C	-2.89899400	-1.48852600	0.81714800
C	-2.24653300	-1.52210400	2.03447600
C	-2.46707700	-0.57427700	3.16268600
C	-1.00106100	-0.61017500	3.93406400
C	-0.13271100	0.70872200	3.84857000
C	1.42730800	0.62471900	3.51485200
C	1.76568400	-0.56665600	2.68775500
C	3.09169400	-0.71609100	1.98193400
C	2.87723500	-2.03552800	1.16397900
C	1.74372000	-2.81749700	1.91020200
C	0.72999300	-3.65491200	1.01150800
C	-0.64306200	-3.06093900	1.12106900
C	-1.12171800	-2.31040300	2.18262400
C	-0.27584900	-1.90233500	3.34263300
C	1.06860300	-1.70118700	2.70469000
F	4.65422100	-1.47765800	-1.13487800
F	3.80247000	-1.13537200	-3.39698000
F	2.51135700	-3.21887000	-3.08490300

F	0.57109400	-2.42627600	-4.49586400
F	-0.97857300	-4.06165100	-3.47381900
F	-2.76202800	-2.35451000	-3.84012000
F	-4.10993000	-2.99514800	-1.74728800
F	-5.28571100	-0.80167200	-1.57470800
F	-5.19472400	-1.19782000	0.82738200
F	-5.23555900	1.06035100	1.61429800
F	-3.73976200	1.39480000	3.57238300
F	2.17124500	2.88850100	3.64689800
F	3.81689100	2.84533300	1.90060300
F	4.92612500	0.70901500	1.61875300
F	3.50949400	4.68207500	-1.46296000
F	1.83356500	4.66963800	0.53277000
F	-4.23613100	3.12248000	0.79978400
F	-4.49315900	2.79399800	-1.56275400
F	-4.26100800	0.83556200	-3.00622700
F	2.46729600	0.64447300	-4.33672900
F	3.42509900	2.47513200	-2.86420000
F	1.13008400	3.40700400	-3.59579700
F	0.81600800	4.95030700	-1.72170200
F	-1.51078100	4.93853100	-0.89277600
F	-2.50385700	3.60292500	-2.84251700
F	1.61090400	-4.80456900	-0.93608500
F	-0.91038000	-5.02870100	-1.26401200
F	-3.38994000	-1.07876900	4.04529700
F	-1.24463400	-0.84696200	5.24870300
F	-0.25428600	1.35755300	5.05687400
F	2.15663500	0.57196400	4.67465700
F	4.01875300	-0.99741400	2.96770300
F	4.03593800	-2.77576200	1.17798500
F	2.33417800	-3.68912600	2.78954500
F	0.74424300	-4.95356600	1.45511500
F	-0.18728500	-2.87273000	4.31730800
O	4.91690300	1.01304700	-0.86392900
H	5.56036400	0.28440300	-0.80988900
H	3.07371300	5.19759900	-0.81351600
IP			
C	3.54327400	-0.13647300	1.36311400
C	3.48934000	1.14906000	0.49793000
C	2.82150700	2.44532100	1.12976400
C	2.09598800	3.14290400	-0.16376000
C	0.67470100	3.76193000	-0.00793500
C	-0.32220800	3.80928400	-1.28430100
C	-1.80437400	3.43358200	-0.64045700

C	-2.79928300	2.47978000	-1.38447900
C	-3.84555200	1.50817700	-0.53376200
C	-3.79671500	0.11443600	-1.32680800
C	-3.94289200	-1.26674500	-0.57374600
C	-2.95242700	-2.46953600	-1.12610500
C	-1.97825200	-2.60636100	-0.01043100
C	-0.71827400	-3.17098900	-0.10005800
C	0.14852100	-3.10149500	0.97647800
C	1.56007000	-3.45694100	0.61103200
C	2.58347100	-2.48664900	1.37702700
C	3.56424300	-1.53143700	0.54161700
C	2.35599800	-0.28014200	2.27383800
C	1.86752400	-1.51513500	2.32037000
C	0.69846600	-1.95997200	3.15927700
C	-0.25958000	-2.47750800	2.14169100
C	-1.51366000	-1.90478800	2.23209700
C	-2.36397400	-1.95114000	1.14314800
C	-3.67788400	-1.26238600	1.00979600
C	-3.72690800	0.07276900	1.84314700
C	-3.56983500	1.43972900	1.01496100
C	-2.18312700	1.86666700	1.33360000
C	-1.41319200	2.76358700	0.62413600
C	-0.08911100	2.94867000	0.96446900
C	0.45845600	2.25805100	2.01938300
C	1.89638200	2.20873700	2.39593300
C	1.94854900	0.83086100	3.18822500
C	0.46899300	0.62118400	3.75205600
C	-0.12160800	-0.82919900	3.93295800
C	-1.69281700	-1.03899100	3.43067100
C	-2.56184600	0.19306500	3.01271400
C	-1.64714700	1.19997400	2.41698800
C	-0.32331800	1.38721600	2.75389000
C	2.83225300	0.98757800	-0.83729600
C	2.10527400	2.04623800	-1.19283300
C	1.56379600	2.30095900	-2.56343600
C	0.10346000	2.92180400	-2.52122100
C	-0.73286400	1.69070100	-2.65474000
C	-1.99366500	1.47557500	-2.12867400
C	-2.52091700	0.19778800	-2.08955600
C	-1.81956800	-0.86086100	-2.63356500
C	-2.15089100	-2.30263800	-2.45626500
C	-0.66953800	-3.02122600	-2.63335700
C	-0.04779400	-3.67279800	-1.33318900
C	1.48571600	-3.42498700	-0.96599400

C	1.98851800	-2.12080900	-1.48152400
C	3.28853100	-1.50995200	-1.01819500
C	3.27185200	-0.11920100	-1.74033900
C	2.32491000	-0.29617500	-2.97550800
C	1.43299400	0.95700400	-3.38814300
C	-0.01576500	0.62903400	-3.18036000
C	-0.57002400	-0.64072700	-3.18017300
C	0.24207800	-1.88802900	-3.29052600
C	1.50141100	-1.51539700	-2.56292300
F	4.82394500	1.46795100	0.22182300
F	3.82349700	3.27363900	1.52744700
F	2.93097900	4.14404300	-0.60391800
F	0.82415700	5.05032100	0.45059700
F	-0.37573100	5.09480300	-1.71154500
F	-2.44301300	4.62395400	-0.39633600
F	-3.56342800	3.23065100	-2.24208700
F	-5.09451200	2.01668300	-0.69085900
F	-4.82938800	0.15820900	-2.24299900
F	-5.22468200	-1.67583600	-0.75980400
F	-3.72430100	-3.60103600	-1.23230700
F	1.84578800	-4.74561100	0.98895400
F	3.37689500	-3.30173500	2.14521400
F	4.83014000	-2.02660800	0.68036400
F	1.10767600	-2.92427900	4.05523400
F	-4.63554100	-2.09054900	1.56219500
F	-4.93694400	0.11297500	2.45729700
F	-4.43473200	2.34430400	1.59867000
F	2.17254900	3.21818900	3.29056800
F	2.83203300	0.92133100	4.22756600
F	0.40268600	1.24635100	4.97737100
F	-0.07898200	-1.12540900	5.25681200
F	-2.34379000	-1.71239500	4.43356700
F	-3.17643800	0.69018900	4.13517900
F	2.41351400	3.16916800	-3.19832300
F	-0.04176600	3.69707200	-3.65038000
F	-2.93361900	-2.74934800	-3.49240400
F	-0.81051100	-4.01194600	-3.55118100
F	-0.22434300	-5.03477100	-1.43441700
F	2.26445800	-4.42666000	-1.48652600
F	4.29274900	-2.25740500	-1.60383900
F	4.54160300	0.18738500	-2.17031200
F	3.09565400	-0.63108100	-4.05962000
F	1.69141300	1.24549200	-4.70470400
F	0.54031800	-2.22825700	-4.59240100

O	4.64848600	-0.06206700	2.22004500
H	5.41950700	0.21056900	1.69166300
C ₁ -S _N 2'-C1-F _k			
RC			
C	-3.10729200	-0.45472700	-0.39845000
C	-3.37623700	1.00749600	-0.50907500
C	-2.88759400	1.71560900	-1.82616100
C	-1.96732100	2.95293600	-1.26349400
C	-0.59381300	3.23272500	-1.93441200
C	0.60248200	3.87749200	-1.05838800
C	1.94947500	3.06953800	-1.58601000
C	3.05277600	2.58981600	-0.58617800
C	3.93895000	1.21932300	-0.89168700
C	4.02240300	0.49872600	0.53989700
C	4.03552800	-1.07404900	0.66449000
C	3.14253600	-1.67276500	1.92129400
C	1.97824400	-2.25879200	1.20848700
C	0.74340200	-2.52730800	1.76109300
C	-0.30247600	-2.92605400	0.95020700
C	-1.60125300	-3.00514700	1.66763800
C	-2.81171900	-2.61562200	0.71443600
C	-3.42495300	-1.15174100	0.89990800
C	-2.62630400	-1.26065900	-1.34072000
C	-2.50881400	-2.69296200	-0.90117200
C	-1.17306000	-3.33993900	-1.39292400
C	-0.10576900	-3.07931000	-0.40047900
C	1.13094700	-2.82125400	-0.95580300
C	2.16261800	-2.37714300	-0.15455300
C	3.49848500	-1.90289400	-0.60311600
C	3.42310800	-1.26081900	-2.03701700
C	3.41096900	0.34344400	-2.09266000
C	1.99215500	0.65563100	-2.40449700
C	1.34929000	1.85764000	-2.19856900
C	-0.01430800	1.94835000	-2.38954200
C	-0.73259300	0.85042500	-2.80663800
C	-2.21636600	0.73335700	-2.87524200
C	-2.38845000	-0.85264600	-2.76035600
C	-1.02835700	-1.45667700	-3.32302100
C	-0.49516900	-2.83364600	-2.77039300
C	1.13602400	-2.85221700	-2.43986900
C	2.07712900	-1.69236300	-2.91331700
C	1.28274100	-0.43838700	-2.85888600
C	-0.08062400	-0.34589000	-3.04226300
C	-2.61991700	1.65428000	0.61146700

C	-1.82707000	2.64297600	0.20346100
C	-1.04342300	3.53727400	1.10474300
C	0.39387300	3.86605300	0.51032100
C	1.22889600	2.82705300	1.18344500
C	2.38190900	2.23940500	0.69479300
C	2.89388300	1.10633600	1.29941500
C	2.29243900	0.59241900	2.43325800
C	2.58494700	-0.73630200	3.04167400
C	1.14718700	-1.09317100	3.79421800
C	0.30936900	-2.27484600	3.16107400
C	-1.27023100	-2.14081900	2.96025300
C	-1.67284400	-0.71890200	2.75636700
C	-3.01130400	-0.34983100	2.18182000
C	-2.89085000	1.22286200	2.02226900
C	-1.73705800	1.65552100	2.99461400
C	-0.77874000	2.83698000	2.50413000
C	0.60833100	2.30157700	2.30412800
C	1.15167100	1.19214900	2.93143300
C	0.37026500	0.29884100	3.83683500
C	-1.00181100	0.33243200	3.22557600
F	-4.72492600	1.24865300	-0.31032800
F	-3.96595700	2.28463000	-2.43304600
F	-2.71425200	4.10379600	-1.37690100
F	-0.81323800	4.06227600	-3.01128200
F	0.72966400	5.17392900	-1.43523200
F	2.54016700	3.86311300	-2.53813100
F	3.95141400	3.61161500	-0.40691100
F	5.19793600	1.61088600	-1.21589000
F	5.19597600	0.93562500	1.12267600
F	5.32705600	-1.44208700	0.86402900
F	3.89936400	-2.65211800	2.51558100
F	-1.81630400	-4.30108100	2.08154300
F	-3.80504300	-3.50438200	0.97629300
F	-4.79414300	-1.28292400	0.95391300
F	-3.53292300	-3.40815000	-1.47345300
F	-1.38434900	-4.69509300	-1.51273200
F	4.32178600	-3.00541500	-0.71987300
F	4.51607200	-1.68158100	-2.72241100
F	4.17410100	0.69703800	-3.18788300
F	-2.66536500	1.10543600	-4.12412900
F	-3.40499500	-1.30788400	-3.55542800
F	-1.17152300	-1.59596300	-4.68693200
F	-0.73358600	-3.77356100	-3.71764600
F	1.62520200	-4.04039800	-2.91973400

F	2.50397300	-1.96197400	-4.18860600
F	-1.74372900	4.70225100	1.27897200
F	0.75306600	5.11135400	0.97665300
F	3.53077100	-0.62585000	4.02994300
F	1.43621100	-1.44093800	5.07400600
F	0.53366100	-3.39320500	3.93172900
F	-1.93559700	-2.64529400	4.04553100
F	-3.96270100	-0.61165500	3.14392800
F	-4.06863900	1.81098700	2.41000800
F	-2.30400200	2.05240300	4.17859000
F	-0.79425600	3.81468500	3.46728700
F	0.31449900	0.76036700	5.13453600
H	-5.94968600	0.76503200	-2.32525300
O	-5.56416100	-0.09912300	-2.52866200
H	-5.45343400	-0.09813300	-3.49056000
TS	imaginary vibrational frequency		-789.61 cm ⁻¹
C	-3.43333200	-0.26312100	-0.82400900
C	-3.33338200	1.26402800	-0.76856900
C	-2.62239200	1.98251800	-1.99627600
C	-1.69705500	3.11432400	-1.28333100
C	-0.25909700	3.37601500	-1.82429000
C	0.88185800	3.90066100	-0.80328900
C	2.23543600	3.05776600	-1.25872200
C	3.21252600	2.46183500	-0.19357800
C	4.05326700	1.06753700	-0.50148700
C	3.97576900	0.26768900	0.88876200
C	3.90503400	-1.30689700	0.92406200
C	2.87840300	-1.92751100	2.06463800
C	1.75948800	-2.42489900	1.22405000
C	0.46972500	-2.66674600	1.65345300
C	-0.51429700	-2.97876200	0.73480200
C	-1.88071600	-2.99759100	1.32830100
C	-2.97436300	-2.48955900	0.28332200
C	-3.65954400	-1.03740300	0.52141500
C	-2.32951600	-0.94773800	-1.47855700
C	-2.46007800	-2.40554600	-1.23968800
C	-1.19743600	-3.17460900	-1.68759400
C	-0.20046300	-3.07082000	-0.59984000
C	1.08572900	-2.82792000	-1.03446500
C	2.05913400	-2.47627500	-0.12286800
C	3.44519500	-2.03709800	-0.43058600
C	3.52202400	-1.31425400	-1.82786700
C	3.59635700	0.28781800	-1.79588000
C	2.23692100	0.70004100	-2.23490700

C	1.64530100	1.92527300	-2.01661300
C	0.31378900	2.10841400	-2.33658100
C	-0.40626300	1.08406200	-2.89795300
C	-1.89242600	1.01088500	-3.00197400
C	-2.03682400	-0.51684700	-2.77262400
C	-0.82973400	-1.19907200	-3.47600900
C	-0.38230900	-2.62545300	-2.96858400
C	1.20843700	-2.75267400	-2.51243400
C	2.24518700	-1.62638000	-2.84554800
C	1.52089500	-0.32777200	-2.82794900
C	0.19419900	-0.14233600	-3.15573600
C	-2.55395400	1.71258300	0.42898100
C	-1.69166600	2.69089200	0.15823100
C	-0.96979300	3.51005200	1.17623600
C	0.52638300	3.81126200	0.73684400
C	1.25116300	2.70049400	1.42174700
C	2.41205800	2.07892500	1.00041800
C	2.81400100	0.89074300	1.58208900
C	2.08952000	0.34900000	2.62734300
C	2.26360500	-1.02329500	3.18121700
C	0.74864900	-1.34457800	3.78253100
C	-0.08275800	-2.44749700	3.01724300
C	-1.62689700	-2.21432800	2.67577900
C	-1.94280700	-0.76975500	2.49714500
C	-3.22076400	-0.29215000	1.85331300
C	-2.98967700	1.26221100	1.78468900
C	-1.91875300	1.58242100	2.88233600
C	-0.86763700	2.73810100	2.55425800
C	0.50763800	2.14864400	2.45177600
C	0.93728500	0.97929600	3.05646000
C	0.03260100	0.07831700	3.82944300
C	-1.27092600	0.21521400	3.09302600
F	-4.60423100	1.78914100	-0.63653400
F	-3.58625400	2.63101300	-2.70377800
F	-2.37935300	4.30798600	-1.36322200
F	-0.35934500	4.29708400	-2.84244000
F	1.10441300	5.20872400	-1.08391000
F	2.95214100	3.88344200	-2.09001300
F	4.13963300	3.42165800	0.12993900
F	5.35409300	1.40917600	-0.69024200
F	5.11173600	0.61366000	1.59465900
F	5.15585100	-1.74982300	1.21265000
F	3.53954900	-2.96785800	2.67014800
F	-2.21767300	-4.29133200	1.66037400

F	-3.99358700	-3.39449100	0.34604400
F	-5.01759000	-1.25938600	0.64386700
F	-3.52658800	-2.94331300	-1.99551100
F	-1.52420500	-4.48997400	-1.92677000
F	4.23004200	-3.16837300	-0.54214100
F	4.65018300	-1.75710800	-2.44015100
F	4.48486300	0.65018100	-2.79022300
F	-2.28465300	1.35346300	-4.27434300
F	-3.47585200	-0.84768200	-3.70911700
F	-1.03566200	-1.27062300	-4.83197400
F	-0.57994600	-3.49469200	-3.99095900
F	1.67345800	-3.93598300	-3.03198100
F	2.77931900	-1.87924900	-4.08407800
F	-1.64814000	4.68972600	1.33856200
F	0.88440200	5.01201000	1.30895200
F	3.11926500	-1.01178300	4.25462300
F	0.90405400	-1.76682000	5.06342400
F	0.00137800	-3.60832900	3.75294300
F	-2.42041300	-2.72233200	3.67192000
F	-4.23326100	-0.52536000	2.76263000
F	-4.16453700	1.91003500	2.07932100
F	-2.57924300	1.93749300	4.03097000
F	-0.93620800	3.66669300	3.56227800
F	-0.13387300	0.47310100	5.13989100
H	-4.25348900	-0.74575800	-2.76120800
O	-4.70736000	-0.49130500	-1.72786000
H	-5.23782200	-1.22329500	-1.35482300
PC			
C	-3.64057000	-0.35213300	-0.64317800
C	-3.32046300	1.13255200	-0.97849400
C	-2.62709600	1.46386500	-2.37105900
C	-1.64232500	2.70704400	-2.01352300
C	-0.22161500	2.77884400	-2.65514300
C	0.96833500	3.51320500	-1.83776500
C	2.28376100	2.53660200	-2.08896200
C	3.27808700	2.20873400	-0.92568100
C	4.07158500	0.75717700	-0.87049500
C	4.02105000	0.35897200	0.68596900
C	3.90548300	-1.14466800	1.14318000
C	2.90092100	-1.39736900	2.43643500
C	1.73163300	-2.04128500	1.78462900
C	0.45062700	-2.10444000	2.29283600
C	-0.57974500	-2.59543700	1.51234900
C	-1.91778000	-2.44296500	2.14330200

C	-3.06105500	-2.20838400	1.05105300
C	-3.69132300	-0.71505300	0.92430700
C	-2.66304900	-1.32913200	-1.22242900
C	-2.66040600	-2.63116900	-0.48348200
C	-1.34816200	-3.44796500	-0.74126700
C	-0.32085100	-3.04323400	0.24199900
C	0.96047000	-2.98553200	-0.26806100
C	1.97913000	-2.45471100	0.49140500
C	3.37037300	-2.18662900	0.04583900
C	3.42704900	-1.86971000	-1.49568700
C	3.55395000	-0.32209100	-1.89986100
C	2.19906500	0.00928700	-2.41879800
C	1.64453900	1.26690400	-2.52156000
C	0.30704800	1.40681200	-2.85335000
C	-0.45926600	0.29762600	-3.11023000
C	-1.95850800	0.22696800	-3.07550400
C	-2.05989600	-1.13256100	-2.38535600
C	-0.95869000	-2.02459500	-2.95608200
C	-0.54578500	-3.29105700	-2.13772100
C	1.04622300	-3.34325600	-1.70343500
C	2.11147500	-2.39837100	-2.36466900
C	1.43813100	-1.11479200	-2.70347000
C	0.11034900	-0.97375800	-3.04168100
C	-2.47150400	1.83898700	0.03280800
C	-1.58966600	2.67640300	-0.51294000
C	-0.81990300	3.72324500	0.22367500
C	0.66465800	3.85001600	-0.32048900
C	1.38452200	2.94000100	0.61860600
C	2.51063100	2.18600900	0.34800300
C	2.90238300	1.18574800	1.21828600
C	2.20418800	0.97307500	2.39307700
C	2.35796700	-0.20700800	3.29075900
C	0.85389500	-0.29890500	3.99752100
C	-0.03844400	-1.53313300	3.57511500
C	-1.59012900	-1.34603700	3.23533300
C	-1.86338300	0.00995900	2.68586300
C	-3.14985100	0.34526300	1.97750600
C	-2.87170500	1.80379200	1.47159000
C	-1.75681100	2.37315500	2.41292900
C	-0.68811100	3.35690200	1.75620600
C	0.66612000	2.71365600	1.78080100
C	1.08656200	1.73762700	2.66883300
C	0.18475300	1.11147100	3.68088200
C	-1.13936100	1.09198100	2.97091900

F	-4.54961800	1.78748900	-0.96036000
F	-3.58176400	1.93506700	-3.21526700
F	-2.29814600	3.86226000	-2.37876000
F	-0.34570500	3.41571700	-3.86880000
F	1.21642300	4.69110800	-2.46238400
F	2.99726600	3.09572800	-3.12091800
F	4.24019800	3.18804800	-0.89360300
F	5.37367600	0.99225800	-1.17636000
F	5.19096800	0.83691400	1.24305000
F	5.15125900	-1.54560000	1.50386700
F	3.54491500	-2.27335400	3.27428000
F	-2.23525200	-3.60600700	2.81005800
F	-4.08765000	-3.01816300	1.42198400
F	-5.02522000	-0.83737100	1.22246300
F	-3.70349100	-3.39632000	-0.94815500
F	-1.64844600	-4.78252500	-0.59098600
F	4.10156800	-3.34437600	0.22548000
F	4.52138200	-2.50438400	-1.98862100
F	4.42810900	-0.27822000	-2.96878100
F	-2.45533000	0.14446800	-4.36370000
F	-3.94206400	-2.21949900	-4.07389400
F	-1.29208200	-2.44578600	-4.25013900
F	-0.80353900	-4.38326200	-2.89927600
F	1.46047700	-4.64192400	-1.86883100
F	2.59882800	-3.01446500	-3.48937400
F	-1.47078500	4.91988500	0.07363800
F	1.07127100	5.14747700	-0.10125000
F	3.25178800	0.05430300	4.29837900
F	1.04334000	-0.37235900	5.33939800
F	0.05602100	-2.46966700	4.57896900
F	-2.35626100	-1.54571900	4.35268800
F	-4.11122000	0.43648800	2.96723800
F	-4.01382200	2.55796200	1.59798000
F	-2.36727400	3.05023200	3.43782800
F	-0.69436800	4.52766100	2.47190600
F	0.07959500	1.84820500	4.84110800
O	-4.86073200	-0.70526600	-1.23980900
H	-5.56664000	-0.18870200	-0.81333600
H	-3.16996300	-2.35860100	-4.58574500
IP			
C	-3.51095700	-0.18650400	-1.40120000
C	-3.27149600	1.32320300	-1.11055900
C	-2.41162700	2.17037500	-2.14654100
C	-1.60089600	3.21155500	-1.20166200

C	-0.11457200	3.55579000	-1.52962400
C	0.87594100	3.96005000	-0.31369300
C	2.29317800	3.18333800	-0.68251300
C	3.13120100	2.46838000	0.42824700
C	4.03075200	1.12393800	0.08035900
C	3.79019700	0.17019500	1.35171200
C	3.73839600	-1.39731400	1.20125500
C	2.58349100	-2.14247200	2.12627000
C	1.57982000	-2.52578000	1.10015700
C	0.24934900	-2.81033500	1.32898400
C	-0.61093100	-2.99769500	0.26249900
C	-2.03470000	-3.12616900	0.67235200
C	-3.02324600	-2.52756100	-0.43240800
C	-3.75528600	-1.11221300	-0.10770600
C	-2.38302300	-0.85126600	-2.13079000
C	-2.36973300	-2.33482700	-1.92551000
C	-0.96764200	-2.96027700	-2.24188300
C	-0.13366100	-2.92672500	-1.02161400
C	1.19778000	-2.64699900	-1.25345000
C	2.04564200	-2.41471500	-0.19416100
C	3.45850600	-1.96423300	-0.27342800
C	3.71115500	-1.09243000	-1.56014200
C	3.76314800	0.49664400	-1.34403100
C	2.47574000	0.96500500	-1.92659500
C	1.83566000	2.15455400	-1.65211000
C	0.55443600	2.37493500	-2.13006000
C	-0.06578600	1.42633800	-2.90514600
C	-1.54510700	1.30453100	-3.13387800
C	-1.62077500	-0.21521600	-3.00775600
C	-0.38634300	-0.80096800	-3.69350400
C	0.01354400	-2.27075700	-3.32923200
C	1.52216600	-2.43977900	-2.68406500
C	2.58688900	-1.28977100	-2.76961800
C	1.86437800	0.01148900	-2.72749300
C	0.59441900	0.23532400	-3.21293100
C	-2.64278400	1.61941000	0.21592700
C	-1.76576900	2.62242100	0.16988100
C	-1.20375000	3.33622200	1.35493500
C	0.32775500	3.69542500	1.14848100
C	0.97896100	2.51864600	1.79536800
C	2.19220200	1.95003000	1.45834700
C	2.53930700	0.70781200	1.95585300
C	1.69908200	0.05215100	2.83730400
C	1.82194700	-1.37389400	3.25326300

C	0.24517400	-1.76319500	3.61647300
C	-0.46831000	-2.77226400	2.63036800
C	-1.96447400	-2.51064400	2.12819800
C	-2.27030100	-1.05492000	2.07546300
C	-3.46464700	-0.51107400	1.33559500
C	-3.24317400	1.03736900	1.45367700
C	-2.32772100	1.23993500	2.70865400
C	-1.26436900	2.42575000	2.64566900
C	0.12249300	1.85582500	2.65882300
C	0.49182200	0.62846700	3.18327000
C	-0.48962400	-0.35474500	3.73026700
C	-1.68968600	-0.14061000	2.85174200
F	-4.54223900	1.89254000	-1.06003500
F	-3.27083400	2.89999100	-2.90638000
F	-2.29411700	4.40226500	-1.22135900
F	-0.11976800	4.60055000	-2.42553600
F	1.10931700	5.29253700	-0.41219900
F	3.09835700	4.10854700	-1.30089200
F	3.98945800	3.38921500	0.97765800
F	5.33823800	1.49086800	0.10398100
F	4.82153800	0.43371700	2.23164300
F	4.94856500	-1.87254500	1.59188600
F	3.17318000	-3.25141300	2.68008700
F	-2.34758600	-4.46125500	0.80443000
F	-4.02069400	-3.44208800	-0.55978200
F	-5.10301900	-1.37188700	-0.10140200
F	-3.26623900	-2.89843300	-2.80503700
F	-1.17364200	-4.26184900	-2.63945500
F	4.25085900	-3.08728900	-0.41035000
F	4.91603900	-1.46936500	-2.05944800
F	4.77858300	0.95829900	-2.15902700
F	-1.86610000	1.68198500	-4.42359600
F	-0.53584400	-0.72494800	-5.06533400
F	-0.03279000	-3.00840900	-4.46561600
F	2.06797000	-3.57272000	-3.23630000
F	3.28490300	-1.43180500	-3.94193900
F	-1.92639200	4.48470100	1.54658500
F	0.58605600	4.82559100	1.89186400
F	2.53392200	-1.48613600	4.42069900
F	0.24409000	-2.32913600	4.84997900
F	-0.44298600	-4.01310400	3.22488800
F	-2.86593100	-3.13291800	2.95023200
F	-4.56409500	-0.82413100	2.11336100
F	-4.45249600	1.65872800	1.65660300

F	-3.13449400	1.46544800	3.79473100
F	-1.47615800	3.24195100	3.72828200
F	-0.82614400	-0.10967600	5.04440400
O	-4.59995000	-0.31769600	-2.27994100
H	-5.40081300	-0.01740600	-1.81565300

C₁-S_N2'-C19-F_r

RC

C	-3.08938600	-0.31350100	-0.47961400
C	-3.27208900	1.11306100	-0.86710600
C	-2.68416100	1.54460200	-2.26243100
C	-1.70851800	2.80705600	-1.87924400
C	-0.28932000	2.87849600	-2.51274300
C	0.91135800	3.59716800	-1.70326300
C	2.22265400	2.62959600	-2.01055500
C	3.24795400	2.26978100	-0.88555300
C	4.05004300	0.81555300	-0.89999100
C	4.02525700	0.35827900	0.63790700
C	3.92644000	-1.16516000	1.03670100
C	2.94431100	-1.47558500	2.33089800
C	1.77286100	-2.10930900	1.67216200
C	0.50141100	-2.19981600	2.19856200
C	-0.53465500	-2.67738100	1.41823300
C	-1.86339200	-2.54576300	2.07021200
C	-3.00157000	-2.25881800	0.99980500
C	-3.51667300	-0.75096100	0.89540900
C	-2.61397100	-1.29580500	-1.23680500
C	-2.63229500	-2.63247400	-0.55691200
C	-1.33685300	-3.44740800	-0.85979900
C	-0.29448300	-3.08220700	0.12752300
C	0.97818100	-2.99997900	-0.40065200
C	2.00436600	-2.48177000	0.36304500
C	3.38644200	-2.17432100	-0.09150500
C	3.41293100	-1.79521200	-1.61754400
C	3.51323000	-0.22844200	-1.95418000
C	2.13337300	0.10830500	-2.38992600
C	1.56796900	1.36527400	-2.43143700
C	0.22257400	1.50191200	-2.70447100
C	-0.54993100	0.39223600	-2.95875700
C	-2.03191500	0.35753700	-3.08485300
C	-2.31773600	-1.16343300	-2.69696000
C	-0.98902800	-1.94739400	-3.08362400
C	-0.57208700	-3.23349600	-2.26841900
C	1.03994800	-3.29190500	-1.85509400
C	2.07799600	-2.29384700	-2.47419900

C	1.37007700	-1.00485800	-2.68364500
C	0.02507000	-0.86526100	-2.95301200
C	-2.52944400	1.91211800	0.16056900
C	-1.65374400	2.76164600	-0.37356100
C	-0.84260600	3.75009000	0.39694900
C	0.63766800	3.87724000	-0.17074100
C	1.37105200	2.92476100	0.71502100
C	2.50116700	2.19219100	0.39875700
C	2.90979700	1.15708900	1.21898200
C	2.22914200	0.89087500	2.39251900
C	2.40669700	-0.32240900	3.23922900
C	0.91835500	-0.45199100	3.96702200
C	0.02896400	-1.67529800	3.50783600
C	-1.52773700	-1.48411200	3.20417800
C	-1.82378400	-0.10000500	2.73289700
C	-3.11019300	0.24036400	2.03678600
C	-2.88096300	1.75182600	1.61000600
C	-1.73813400	2.27903400	2.54928900
C	-0.68155100	3.29327400	1.90910200
C	0.67099700	2.64594000	1.87614400
C	1.11243900	1.63717200	2.71681500
C	0.23678900	0.96966900	3.72434600
C	-1.10375700	0.97640300	3.04591800
F	-4.61502200	1.43024300	-0.80207000
F	-3.70289400	2.03950100	-3.00923600
F	-2.36926500	3.95920300	-2.23782100
F	-0.40553300	3.51324100	-3.72861900
F	1.14104100	4.79593200	-2.29379300
F	2.90395100	3.20570100	-3.05372000
F	4.20658100	3.25053600	-0.83760100
F	5.34491100	1.06671700	-1.22165500
F	5.20051000	0.82127000	1.19663700
F	5.18073200	-1.56798400	1.36460900
F	3.60722300	-2.37743300	3.12601600
F	-2.18855200	-3.72973300	2.69408000
F	-4.06654500	-3.02647800	1.35494100
F	-4.90032100	-0.79098000	0.89993600
F	-3.69464500	-3.35968400	-1.06137600
F	-1.64443000	-4.78529100	-0.75420200
F	4.13788200	-3.32624200	0.03107600
F	4.50108800	-2.39720100	-2.16076600
F	4.34426200	-0.12422500	-3.05182400
F	-2.39417200	0.52494800	-4.40077500
F	-3.35938200	-1.67070900	-3.42229200

F	-1.09513000	-2.32244400	-4.40465500
F	-0.83601900	-4.31221600	-3.04545200
F	1.46368200	-4.57425000	-2.09471500
F	2.53758500	-2.81420900	-3.65684500
F	-1.46326000	4.96988100	0.33155500
F	1.06444900	5.16031500	0.09097800
F	3.31678000	-0.09426800	4.24053600
F	1.13060400	-0.58212300	5.30114700
F	0.14400900	-2.64969000	4.47325000
F	-2.27134900	-1.74609500	4.32400700
F	-4.11615100	0.20596300	2.97853000
F	-4.03240700	2.46366800	1.83474600
F	-2.32228700	2.91285000	3.61594100
F	-0.66527700	4.42403000	2.68670000
F	0.15996400	1.65735300	4.91615500
H	-5.58614600	-1.93845400	-1.98650000
O	-5.68492100	-0.97478300	-1.96743600
H	-6.12324100	-0.79787200	-1.12220000
TS	imaginary vibrational frequency -815.93 cm ⁻¹		
C	-2.78304900	-0.27694100	-0.44626700
C	-2.98749600	0.98901400	-1.01133800
C	-2.56749300	1.34288900	-2.45310400
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C	2.32089600	2.31331400	-2.25734100
C	3.31624400	2.05380700	-1.08298200
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C	3.84689400	-1.15623800	1.23202200
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C	2.14937500	-0.23300100	-2.34311700
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C	-1.98172300	0.07824900	-3.16365000
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C	1.35010800	-1.34606800	-2.51277700
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C	0.74805200	3.82098500	-0.60656800
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F	4.42531100	-2.77299700	-1.78719300
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C₁-S_N2'-C19-F_i

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C	2.40669700	-0.32240900	3.23922900
C	0.91835500	-0.45199100	3.96702200
C	0.02896400	-1.67529800	3.50783600
C	-1.52773700	-1.48411200	3.20417800
C	-1.82378400	-0.10000500	2.73289700
C	-3.11019300	0.24036400	2.03678600
C	-2.88096300	1.75182600	1.61000600
C	-1.73813400	2.27903400	2.54928900
C	-0.68155100	3.29327400	1.90910200
C	0.67099700	2.64594000	1.87614400
C	1.11243900	1.63717200	2.71681500
C	0.23678900	0.96966900	3.72434600
C	-1.10375700	0.97640300	3.04591800
F	-4.61502200	1.43024300	-0.80207000
F	-3.70289400	2.03950100	-3.00923600
F	-2.36926500	3.95920300	-2.23782100
F	-0.40553300	3.51324100	-3.72861900
F	1.14104100	4.79593200	-2.29379300
F	2.90395100	3.20570100	-3.05372000
F	4.20658100	3.25053600	-0.83760100
F	5.34491100	1.06671700	-1.22165500
F	5.20051000	0.82127000	1.19663700
F	5.18073200	-1.56798400	1.36460900
F	3.60722300	-2.37743300	3.12601600
F	-2.18855200	-3.72973300	2.69408000
F	-4.06654500	-3.02647800	1.35494100
F	-4.90032100	-0.79098000	0.89993600
F	-3.69464500	-3.35968400	-1.06137600
F	-1.64443000	-4.78529100	-0.75420200
F	4.13788200	-3.32624200	0.03107600
F	4.50108800	-2.39720100	-2.16076600

F	4.34426200	-0.12422500	-3.05182400
F	-2.39417200	0.52494800	-4.40077500
F	-3.35938200	-1.67070900	-3.42229200
F	-1.09513000	-2.32244400	-4.40465500
F	-0.83601900	-4.31221600	-3.04545200
F	1.46368200	-4.57425000	-2.09471500
F	2.53758500	-2.81420900	-3.65684500
F	-1.46326000	4.96988100	0.33155500
F	1.06444900	5.16031500	0.09097800
F	3.31678000	-0.09426800	4.24053600
F	1.13060400	-0.58212300	5.30114700
F	0.14400900	-2.64969000	4.47325000
F	-2.27134900	-1.74609500	4.32400700
F	-4.11615100	0.20596300	2.97853000
F	-4.03240700	2.46366800	1.83474600
F	-2.32228700	2.91285000	3.61594100
F	-0.66527700	4.42403000	2.68670000
F	0.15996400	1.65735300	4.91615500
H	-5.58614600	-1.93845400	-1.98650000
O	-5.68492100	-0.97478300	-1.96743600
H	-6.12324100	-0.79787200	-1.12220000
TS	imaginary vibrational frequency		-731.84 cm ⁻¹
C	-2.81467200	-0.23987700	-0.48443500
C	-3.10945600	1.13903900	-0.95868100
C	-2.56927700	1.53497500	-2.36646500
C	-1.58014300	2.80097200	-2.04844300
C	-0.15004600	2.77099600	-2.64918500
C	1.06229000	3.48437200	-1.86002900
C	2.33485500	2.44837300	-2.09247100
C	3.32814700	2.11034300	-0.93476500
C	4.07168300	0.62712300	-0.86244100
C	4.00421700	0.25148700	0.69542300
C	3.84512800	-1.24488600	1.16699600
C	2.83103400	-1.45150700	2.45711600
C	1.64791000	-2.06945800	1.80672700
C	0.36557300	-2.08000200	2.31244000
C	-0.67306900	-2.54422600	1.53125900
C	-2.00014600	-2.35505400	2.15438000
C	-3.09641400	-2.06826700	1.05443000
C	-3.30150000	-0.55913500	0.79447500
C	-3.03335000	-1.36478700	-1.35887400
C	-2.82906100	-2.64387400	-0.48095400
C	-1.46638700	-3.40766100	-0.72254300
C	-0.43678400	-2.99850400	0.25909900

C	0.84779600	-3.01655500	-0.24006000
C	1.88431600	-2.51462200	0.52134300
C	3.28548000	-2.29006800	0.07988800
C	3.34954500	-1.99118600	-1.46315900
C	3.50957400	-0.44817400	-1.87242400
C	2.14664300	-0.08502400	-2.33763600
C	1.63237000	1.18903400	-2.44748700
C	0.29794500	1.36244100	-2.74161300
C	-0.51520500	0.26835400	-2.94097000
C	-1.98272700	0.30051800	-3.13464400
C	-2.41005100	-1.23013600	-2.76612800
C	-1.04159800	-2.05603900	-2.98961200
C	-0.68393000	-3.30755300	-2.11575000
C	0.92289300	-3.40466200	-1.67083500
C	2.00723000	-2.48208800	-2.31772400
C	1.34384800	-1.18119100	-2.58371100
C	0.00276500	-1.00451200	-2.85927000
C	-2.47149300	2.05540100	0.02004100
C	-1.56847700	2.85891900	-0.54052100
C	-0.72246300	3.83611300	0.19955600
C	0.77464600	3.85716800	-0.34857400
C	1.44813200	2.91589300	0.59452500
C	2.55582500	2.12711300	0.33714900
C	2.90877100	1.11833800	1.21379900
C	2.19712700	0.93738200	2.38508800
C	2.31864400	-0.23418400	3.29685800
C	0.81424000	-0.27093300	4.00457600
C	-0.11079200	-1.48130300	3.58873600
C	-1.65871000	-1.25174100	3.25309000
C	-1.90697900	0.12629600	2.72838800
C	-3.14109800	0.46005400	1.92618700
C	-2.85601500	1.95470400	1.46536400
C	-1.71667300	2.48666000	2.40574300
C	-0.60663600	3.42670400	1.73445700
C	0.71592600	2.72001000	1.75216600
C	1.10261000	1.73842200	2.64967000
C	0.18952900	1.16195200	3.68073400
C	-1.14747200	1.18919400	2.99265100
F	-4.50407500	1.35454600	-0.99647700
F	-3.60398200	2.01259500	-3.11815200
F	-2.19604700	3.93799100	-2.51813900
F	-0.20848700	3.32703600	-3.90839000
F	1.35051700	4.63907800	-2.51034500
F	3.05196900	2.93187700	-3.15877000

F	4.32423300	3.05432900	-0.92158300
F	5.38048100	0.80919400	-1.17469900
F	5.18640300	0.70078700	1.25135700
F	5.07858200	-1.67578400	1.53600200
F	3.44548500	-2.33560000	3.30914000
F	-2.36833200	-3.50456600	2.81718000
F	-4.22897000	-2.67300100	1.50294500
F	-5.05092700	-0.59790600	0.58044200
F	-3.81225800	-3.54965200	-0.74237000
F	-1.74140300	-4.74600700	-0.52419500
F	3.98918900	-3.46207200	0.27390100
F	4.42220900	-2.65807900	-1.95876500
F	4.35411600	-0.42442500	-2.96472800
F	-2.27054400	0.46721700	-4.47233900
F	-3.31432800	-1.66000400	-3.69891400
F	-1.07100600	-2.48347900	-4.30100300
F	-0.98255400	-4.41354700	-2.84192200
F	1.29523700	-4.71447500	-1.82747900
F	2.46314700	-3.06617400	-3.47157200
F	-1.26427900	5.08986900	0.08287900
F	1.26618100	5.12855200	-0.14711100
F	3.22103900	0.01420000	4.30062900
F	1.00075000	-0.34303100	5.34713200
F	-0.04331100	-2.41393200	4.59910900
F	-2.42304400	-1.45368800	4.37066200
F	-4.23406100	0.43935100	2.75616700
F	-3.99189200	2.70317500	1.64448500
F	-2.29925700	3.20373400	3.42003100
F	-0.54738700	4.58555100	2.46857300
F	0.13908000	1.91448200	4.83489600
H	-5.02406700	-1.04204100	-0.61590500
O	-4.65947900	-1.41760800	-1.61063800
H	-4.88879200	-0.74721000	-2.28388300
PC			
C	-3.04592800	-0.26169600	-0.50882500
C	-3.23767400	1.15877400	-0.94078300
C	-2.64545300	1.52643600	-2.34621100
C	-1.64283600	2.79008800	-2.01500900
C	-0.21419900	2.78597700	-2.62512100
C	0.99971300	3.51133800	-1.84262500
C	2.28583600	2.49650700	-2.09686400
C	3.30128400	2.16246500	-0.95367800
C	4.06827900	0.68850200	-0.89977900
C	4.02388100	0.29865900	0.65602300

C	3.88745300	-1.20392400	1.11901900
C	2.89193700	-1.43475000	2.41976900
C	1.70802900	-2.06642700	1.78165900
C	0.43271900	-2.10675400	2.30612300
C	-0.60918200	-2.59138100	1.53849900
C	-1.94145000	-2.40729500	2.16193900
C	-2.97858200	-2.05895000	1.03683700
C	-3.01925500	-0.58145300	0.78268000
C	-3.16810400	-1.44942900	-1.41790400
C	-2.78603500	-2.68628200	-0.46943000
C	-1.41531700	-3.42969900	-0.72805300
C	-0.38138500	-3.02078100	0.25356400
C	0.89779500	-3.01027500	-0.26197000
C	1.93561100	-2.49737600	0.48990700
C	3.32834500	-2.24765900	0.03215700
C	3.37180300	-1.93506400	-1.50864200
C	3.50731000	-0.38592700	-1.90854800
C	2.13219600	-0.03602800	-2.34693800
C	1.59536700	1.23000800	-2.44570000
C	0.25364900	1.38549600	-2.71832700
C	-0.55092100	0.28259500	-2.90080200
C	-2.02091900	0.28942700	-3.10936800
C	-2.40080400	-1.26146500	-2.77687700
C	-1.01929400	-2.05097600	-2.98431300
C	-0.64450800	-3.30416300	-2.12456600
C	0.96474900	-3.38296900	-1.69769000
C	2.02587900	-2.43530900	-2.34697100
C	1.34086300	-1.14015100	-2.58251700
C	-0.00632800	-0.97943800	-2.82960900
C	-2.50400200	2.01211900	0.05450500
C	-1.60474800	2.81540200	-0.50787000
C	-0.76263600	3.80080300	0.23530400
C	0.72554400	3.86051800	-0.32534000
C	1.42881900	2.92505300	0.60308200
C	2.54591500	2.15663500	0.32803600
C	2.92356900	1.14678900	1.19357800
C	2.22952300	0.94627100	2.37260800
C	2.37765700	-0.23065700	3.27433500
C	0.88500500	-0.29391100	4.00349300
C	-0.03205200	-1.51840000	3.59216900
C	-1.58847700	-1.30723600	3.28535200
C	-1.85540200	0.08493900	2.80089500
C	-3.03933000	0.38616900	1.93083400
C	-2.83538800	1.89230200	1.51333500

C	-1.70024500	2.44432900	2.45042900
C	-0.61654600	3.39598500	1.76831300
C	0.71581900	2.71026300	1.76917200
C	1.12859400	1.73065800	2.65803700
C	0.24396300	1.14029200	3.70738900
C	-1.10671600	1.15847900	3.05170100
F	-4.58455300	1.44989300	-0.92811100
F	-3.65240200	2.00869000	-3.12080700
F	-2.26934200	3.93401500	-2.44924700
F	-0.28791400	3.34524900	-3.88105200
F	1.26286500	4.67639800	-2.48389400
F	2.98204900	2.99637500	-3.16888200
F	4.28338700	3.12048700	-0.94608900
F	5.37020400	0.89153600	-1.22614300
F	5.20686200	0.75743400	1.20179500
F	5.13037200	-1.62210500	1.47029900
F	3.52898300	-2.31741300	3.25649800
F	-2.35411300	-3.55291400	2.79924200
F	-4.22300400	-2.48142800	1.48717900
F	-5.96306500	-0.46661400	0.66311300
F	-3.75757100	-3.62947800	-0.64819400
F	-1.66197600	-4.77728900	-0.54465900
F	4.04928300	-3.41189000	0.20832600
F	4.44704100	-2.58405700	-2.02168300
F	4.33433300	-0.34362600	-3.01309600
F	-2.28603200	0.47541400	-4.44828000
F	-3.24260900	-1.71557000	-3.76611900
F	-0.99592000	-2.46726500	-4.30237800
F	-0.93756100	-4.40751600	-2.85914000
F	1.35772100	-4.68467500	-1.87019000
F	2.47165800	-2.99504500	-3.51665400
F	-1.33735700	5.04028700	0.12677400
F	1.18995700	5.14035400	-0.11447800
F	3.29089500	0.02166400	4.26711400
F	1.09316500	-0.37934400	5.34199200
F	0.06609800	-2.45523900	4.59614000
F	-2.32933500	-1.54649600	4.41021000
F	-4.20843400	0.23875700	2.64565900
F	-3.99528600	2.58738300	1.73635700
F	-2.29378700	3.15889300	3.45983400
F	-0.56389100	4.55869900	2.49704600
F	0.22245200	1.88239600	4.86881000
O	-4.54731700	-1.49844700	-1.69059000
H	-4.68559400	-2.04438800	-2.48456900

H	-5.72476300	-1.36638600	0.76119200
IP			
C	-3.12969300	-0.48106200	-0.29232300
C	-3.43291100	0.90649100	-0.76065500
C	-2.95694200	1.25592900	-2.21254900
C	-2.01828000	2.59151300	-1.99070500
C	-0.63155200	2.65112800	-2.68781200
C	0.57841300	3.47879200	-2.00697400
C	1.90893100	2.53569600	-2.30549000
C	3.00911500	2.30802700	-1.21575400
C	3.86985400	0.88734500	-1.15855900
C	3.94320900	0.55535800	0.40975500
C	3.92994200	-0.93330400	0.93214300
C	3.03102600	-1.17417400	2.29949500
C	1.85359900	-1.90073100	1.75868000
C	0.61764500	-1.99918500	2.36306600
C	-0.43565200	-2.57570100	1.67919800
C	-1.73647900	-2.45055000	2.37697300
C	-2.86790800	-2.21466200	1.31326900
C	-3.00884200	-0.75053700	1.00558500
C	-3.23354300	-1.70664500	-1.15115900
C	-2.72320600	-2.88178400	-0.18556800
C	-1.32423600	-3.54757600	-0.50223000
C	-0.26005000	-3.03811700	0.39748100
C	0.98311000	-2.97047500	-0.19628300
C	2.02984900	-2.36665000	0.47103300
C	3.37392200	-2.05015500	-0.08115100
C	3.30553700	-1.79535300	-1.63161400
C	3.31936000	-0.25726400	-2.09360000
C	1.90156900	-0.00925200	-2.45966600
C	1.28076500	1.21700900	-2.56935300
C	-0.08228800	1.27937300	-2.76307100
C	-0.82485800	0.12300000	-2.85483600
C	-2.30247400	0.03106400	-2.97070800
C	-2.56169400	-1.52639600	-2.56166000
C	-1.14856400	-2.23673000	-2.82615900
C	-0.64585000	-3.43055500	-1.94707000
C	0.98778300	-3.39380700	-1.61924500
C	1.94630000	-2.40924500	-2.36638100
C	1.16867500	-1.16801800	-2.60538800
C	-0.19819700	-1.09974200	-2.77331300
C	-2.69948700	1.84247700	0.15463500
C	-1.89131400	2.67922200	-0.49057200
C	-1.07089700	3.74158400	0.16524000

C	0.37455700	3.86962900	-0.48867700
C	1.18904800	3.01504600	0.42663900
C	2.33366400	2.30566100	0.10950000
C	2.82547000	1.35537500	0.98502600
C	2.21650600	1.15797800	2.21069900
C	2.49312600	0.02825800	3.14199200
C	1.05400000	-0.09797600	3.96435900
C	0.19395300	-1.39092000	3.65440600
C	-1.38941400	-1.28921200	3.43887300
C	-1.77729600	0.06585400	2.92862600
C	-3.02178500	0.26078800	2.11439800
C	-2.93569000	1.75933500	1.63323700
C	-1.78759400	2.41579300	2.48014100
C	-0.80857500	3.40474600	1.69957300
C	0.56169100	2.80230800	1.64143700
C	1.08650000	1.88327900	2.53576500
C	0.30603800	1.28095800	3.65828300
C	-1.08146900	1.19170700	3.09003500
F	-4.79744700	1.11283900	-0.66737600
F	-4.03976000	1.64541800	-2.93551300
F	-2.74183000	3.67633300	-2.42588700
F	-0.81601400	3.15777700	-3.95473900
F	0.72807400	4.63227500	-2.70357200
F	2.50835400	3.03806900	-3.43327800
F	3.92669600	3.32442000	-1.30219000
F	5.13462300	1.15777900	-1.57110700
F	5.12540900	1.10660700	0.86420800
F	5.21574600	-1.26107700	1.21972100
F	3.77197800	-1.98270000	3.12553300
F	-2.03158100	-3.59419100	3.07978100
F	-4.03927800	-2.68359900	1.85376700
F	-3.64149200	-3.88738900	-0.27832400
F	-1.47158000	-4.89947400	-0.25551800
F	4.17728200	-3.15996000	0.08997400
F	4.38723600	-2.39674100	-2.18726300
F	4.07657700	-0.20734500	-3.24689500
F	-2.66024300	0.15161200	-4.29547200
F	-3.43080100	-2.06916200	-3.47903900
F	-1.17596800	-2.70155100	-4.12807900
F	-0.91125400	-4.57735700	-2.62354700
F	1.45279900	-4.67438000	-1.77063000
F	2.35564200	-2.98567000	-3.54148300
F	-1.72861200	4.93833200	0.04954200
F	0.76871600	5.18262600	-0.35219800

F	3.44633000	0.37498700	4.06633900
F	1.34692200	-0.11747300	5.28974400
F	0.41142100	-2.27993900	4.68281700
F	-2.04223600	-1.53209900	4.61635900
F	-4.15318100	0.07341400	2.88427000
F	-4.12509200	2.39022100	1.89920300
F	-2.36717400	3.13210800	3.49654300
F	-0.78697200	4.59556900	2.38317000
F	0.30762400	2.06632600	4.79153400
O	-4.62104700	-1.83381900	-1.34003500
H	-4.77834700	-2.45855300	-2.06937200

M06-PCM/6-31G(d)

C₁ isomer

C	-3.00197100	-0.43913300	-1.00730000
C	-3.25706700	1.00905000	-1.19343900
C	-2.53108300	1.70556300	-2.39284700
C	-1.73693200	2.93589400	-1.67718300
C	-0.26797800	3.20935800	-2.06446700
C	0.73428300	3.85510100	-0.98733900
C	2.14554200	3.04277400	-1.23963800
C	3.03965900	2.56109600	-0.06115400
C	3.95573000	1.19268600	-0.18544300
C	3.75891800	0.48661900	1.22949500
C	3.74392100	-1.07395100	1.36707500
C	2.62803900	-1.65559000	2.42404200
C	1.61060400	-2.20549600	1.50411100
C	0.29874200	-2.46789000	1.81190100
C	-0.56737500	-2.87336900	0.82466300
C	-1.96633100	-2.97267500	1.28848400
C	-2.96299000	-2.59248100	0.12535200
C	-3.58833800	-1.13146100	0.18587100
C	-2.34150100	-1.24445800	-1.82359600
C	-2.35086800	-2.67230600	-1.38893800
C	-0.96664000	-3.32796200	-1.62433500
C	-0.11787200	-3.04103400	-0.45669900
C	1.19456600	-2.78765200	-0.76700300
C	2.04604800	-2.32998500	0.20891100
C	3.44870300	-1.89937400	0.03437700
C	3.65833600	-1.28244800	-1.38298500
C	3.65659000	0.30995300	-1.44421500
C	2.31931700	0.61860000	-1.98772000
C	1.66249100	1.82237900	-1.91782100
C	0.36878400	1.91630100	-2.36310900
C	-0.25578700	0.82243100	-2.90155000

C	-1.68181600	0.71804000	-3.27457300
C	-1.87916100	-0.84986000	-3.17964500
C	-0.46214500	-1.46438300	-3.48756400
C	-0.04675400	-2.83336400	-2.84436000
C	1.48502200	-2.85347000	-2.21353900
C	2.50874600	-1.71108900	-2.49006400
C	1.71363800	-0.46739100	-2.57071900
C	0.41720500	-0.37169000	-3.01171300
C	-2.72927500	1.65080700	0.03894200
C	-1.86260500	2.62213100	-0.21706100
C	-1.27920200	3.52593600	0.80587400
C	0.23078300	3.84833400	0.50122900
C	0.90924200	2.80202000	1.30669000
C	2.12708000	2.21086500	1.05122900
C	2.50373800	1.08337100	1.74163800
C	1.70292400	0.58469700	2.74548300
C	1.87158200	-0.72819200	3.41533300
C	0.32007300	-1.06856600	3.87747600
C	-0.38568000	-2.23860500	3.10213300
C	-1.88539000	-2.10976600	2.60605000
C	-2.22544100	-0.69477100	2.30962200
C	-3.42948200	-0.32758400	1.50732500
C	-3.27348800	1.23205400	1.36243800
C	-2.33315100	1.67001700	2.52686600
C	-1.29911400	2.83894700	2.22361100
C	0.08738100	2.28943600	2.28607400
C	0.49812700	1.19027000	3.01205100
C	-0.43748300	0.31678500	3.76143100
C	-1.65609000	0.35306800	2.89449100
F	-4.60455300	1.21564500	-1.27728500
F	-3.47358000	2.24407200	-3.18874700
F	-2.44180100	4.07488200	-1.91433200
F	-0.25755700	4.00342600	-3.16956500
F	0.93357100	5.13686000	-1.33683000
F	2.88896100	3.80589500	-2.08138100
F	3.88121700	3.56266300	0.30032900
F	5.24318300	1.57233000	-0.26927200
F	4.77107900	0.93676200	2.02915600
F	4.96048300	-1.44392800	1.80578100
F	3.23240700	-2.65037800	3.12298500
F	-2.23166400	-4.25880200	1.65099000
F	-3.98223300	-3.46922200	0.18797100
F	-4.92592000	-1.24745100	-0.04891800
F	-3.25385500	-3.33273600	-2.16377000

F	-1.14620500	-4.66978200	-1.76069400
F	4.22980100	-3.01803100	0.09551600
F	4.84916100	-1.70755600	-1.83965500
F	4.57614900	0.65565400	-2.39323800
F	-1.85172900	1.07287600	-4.57779400
F	-2.78292600	-1.29160800	-4.08701000
F	-0.34650300	-1.58944000	-4.83846300
F	-0.10379400	-3.76908000	-3.80549600
F	2.03303100	-4.04569100	-2.55829100
F	3.16049300	-1.95796300	-3.65347200
F	-1.99682600	4.67576800	0.81850900
F	0.49841200	5.07091000	1.03888100
F	2.60278800	-0.60475600	4.55192100
F	0.35236100	-1.40412600	5.17900700
F	-0.30001200	-3.35627700	3.87495300
F	-2.74471300	-2.59177700	3.53631300
F	-4.52922900	-0.57371700	2.27333300
F	-4.49036400	1.81783600	1.49424000
F	-3.11035100	2.05740400	3.56897600
F	-1.47830400	3.81290700	3.15170700
F	-0.73884500	0.79403700	5.00081000

C₁-S_N2'-C60-F_a

RC

C	-2.66045000	-1.45199100	0.98614300
C	-2.78084900	-2.29804000	-0.22443100
C	-1.76014200	-3.47643500	-0.36267400
C	-1.07528300	-3.20351600	-1.81426600
C	0.45764400	-3.32013100	-1.95582900
C	1.22609900	-2.43118600	-3.05048700
C	2.60616900	-1.97295400	-2.27265800
C	3.17683100	-0.53209900	-2.39334000
C	4.01031900	0.16617900	-1.14877400
C	3.45043800	1.65582000	-1.11989400
C	3.31106400	2.45501600	0.22088200
C	1.95178900	3.37257500	0.33524100
C	1.13870200	2.58792100	1.28741500
C	-0.22504200	2.67166000	1.44736700
C	-0.85699900	1.77272500	2.27561500
C	-2.32546200	1.87790500	2.22034800
C	-3.00946700	0.47474100	2.42709900
C	-3.54223300	-0.24689400	1.11381800
C	-1.88679200	-1.66579000	2.03838700
C	-2.07964600	-0.66556600	3.13013900
C	-0.72082000	-0.26329600	3.75728400

C	-0.14036700	0.83060400	2.95979500
C	1.22116100	0.75569000	2.81182500
C	1.85169200	1.61074100	1.93980400
C	3.27969800	1.58655600	1.55716900
C	3.83928800	0.12846000	1.60829800
C	3.95057000	-0.61696900	0.20425000
C	2.79429300	-1.53382400	0.22402500
C	2.21566600	-2.14729500	-0.85890900
C	1.06839100	-2.87888300	-0.69137300
C	0.51637300	-3.02003300	0.55455300
C	-0.79409700	-3.62448200	0.87187900
C	-1.10303500	-2.90989300	2.25132400
C	0.30701500	-2.58226300	2.87541800
C	0.48016600	-1.32849800	3.80459000
C	1.82419500	-0.41573000	3.48173800
C	2.94952300	-0.91665300	2.52762000
C	2.27153100	-1.71116100	1.48144300
C	1.12054100	-2.44114100	1.64599000
C	-2.51416100	-1.38275700	-1.36598600
C	-1.55335900	-1.82735400	-2.16584700
C	-1.16254100	-1.19274800	-3.44840900
C	0.39590900	-1.24941700	-3.67240100
C	0.80769400	0.06147100	-3.11201500
C	2.01238300	0.37406400	-2.51942000
C	2.15013500	1.54712900	-1.81756500
C	1.11139700	2.44719500	-1.76336500
C	1.04646200	3.64504500	-0.89484700
C	-0.58815600	3.85143400	-0.72778800
C	-1.18503800	3.52505300	0.69650200
C	-2.51019200	2.66456400	0.87234100
C	-2.67177200	1.72633400	-0.26418700
C	-3.63733100	0.59355600	-0.18903800
C	-3.36713200	-0.16968300	-1.53720400
C	-2.69198800	0.87471500	-2.48144600
C	-1.54581000	0.33694100	-3.44622900
C	-0.24635000	0.94507000	-3.03732400
C	-0.08046500	2.14055400	-2.37037200
C	-1.21052700	2.97284500	-1.89127000
C	-2.20264600	1.92653400	-1.49034500
F	-4.06100900	-2.76906100	-0.30378200
F	-2.46345500	-4.61982700	-0.46077500
F	-1.63196800	-4.07124900	-2.70240600
F	0.76301500	-4.62476600	-2.19402000
F	1.57773200	-3.24737800	-4.05814200

F	3.56755000	-2.86693700	-2.62139400
F	3.97326500	-0.45548700	-3.48952200
F	5.30487700	0.22999800	-1.50929600
F	4.27464400	2.38946400	-1.92562300
F	4.37117900	3.27995300	0.30204300
F	2.32262300	4.55967300	0.88178500
F	-2.74662000	2.69113700	3.23120900
F	-4.06954800	0.67587900	3.23234200
F	-4.79613700	-0.71095000	1.38104100
F	-2.82140400	-1.25648800	4.10702200
F	-0.94826600	0.15695100	5.03213600
F	3.96800900	2.30009400	2.49794000
F	5.07469600	0.18894900	2.13525200
F	5.08044700	-1.38281300	0.26219900
F	-0.64678600	-4.95419000	1.12389900
F	-1.79872000	-3.72537600	3.07904800
F	0.72082400	-3.67687100	3.57202900
F	0.58382800	-1.77094700	5.06860200
F	2.36269700	-0.08082400	4.68133300
F	3.83387000	-1.67294800	3.22532400
F	-1.79272400	-1.84518400	-4.45589000
F	0.61005700	-1.25077600	-5.01745600
F	1.51604700	4.73884500	-1.55012100
F	-0.83022800	5.14768100	-0.99538300
F	-1.37326900	4.70881000	1.34446700
F	-3.62509900	3.42566300	0.99808000
F	-4.89155000	1.12486900	-0.23854700
F	-4.54784500	-0.58486100	-2.06268600
F	-3.65731800	1.43308500	-3.25263000
F	-1.86456900	0.68208100	-4.72042800
F	-1.69690700	3.75615600	-2.89362300
H	-3.80682900	5.17675100	-0.47590200
O	-3.54220200	4.69392800	-1.26893400
H	-3.12291500	5.35609600	-1.83252800
TS	imaginary vibrational frequency		-807.08 cm ⁻¹
C	-2.66045000	-1.45199100	0.98614300
C	-2.78084900	-2.29804000	-0.22443100
C	-1.76014200	-3.47643500	-0.36267400
C	-1.07528300	-3.20351600	-1.81426600
C	0.45764400	-3.32013100	-1.95582900
C	1.22609900	-2.43118600	-3.05048700
C	2.60616900	-1.97295400	-2.27265800
C	3.17683100	-0.53209900	-2.39334000
C	4.01031900	0.16617900	-1.14877400

C	3.45043800	1.65582000	-1.11989400
C	3.31106400	2.45501600	0.22088200
C	1.95178900	3.37257500	0.33524100
C	1.13870200	2.58792100	1.28741500
C	-0.22504200	2.67166000	1.44736700
C	-0.85699900	1.77272500	2.27561500
C	-2.32546200	1.87790500	2.22034800
C	-3.00946700	0.47474100	2.42709900
C	-3.54223300	-0.24689400	1.11381800
C	-1.88679200	-1.66579000	2.03838700
C	-2.07964600	-0.66556600	3.13013900
C	-0.72082000	-0.26329600	3.75728400
C	-0.14036700	0.83060400	2.95979500
C	1.22116100	0.75569000	2.81182500
C	1.85169200	1.61074100	1.93980400
C	3.27969800	1.58655600	1.55716900
C	3.83928800	0.12846000	1.60829800
C	3.95057000	-0.61696900	0.20425000
C	2.79429300	-1.53382400	0.22402500
C	2.21566600	-2.14729500	-0.85890900
C	1.06839100	-2.87888300	-0.69137300
C	0.51637300	-3.02003300	0.55455300
C	-0.79409700	-3.62448200	0.87187900
C	-1.10303500	-2.90989300	2.25132400
C	0.30701500	-2.58226300	2.87541800
C	0.48016600	-1.32849800	3.80459000
C	1.82419500	-0.41573000	3.48173800
C	2.94952300	-0.91665300	2.52762000
C	2.27153100	-1.71116100	1.48144300
C	1.12054100	-2.44114100	1.64599000
C	-2.51416100	-1.38275700	-1.36598600
C	-1.55335900	-1.82735400	-2.16584700
C	-1.16254100	-1.19274800	-3.44840900
C	0.39590900	-1.24941700	-3.67240100
C	0.80769400	0.06147100	-3.11201500
C	2.01238300	0.37406400	-2.51942000
C	2.15013500	1.54712900	-1.81756500
C	1.11139700	2.44719500	-1.76336500
C	1.04646200	3.64504500	-0.89484700
C	-0.58815600	3.85143400	-0.72778800
C	-1.18503800	3.52505300	0.69650200
C	-2.51019200	2.66456400	0.87234100
C	-2.67177200	1.72633400	-0.26418700
C	-3.63733100	0.59355600	-0.18903800

C	-3.36713200	-0.16968300	-1.53720400
C	-2.69198800	0.87471500	-2.48144600
C	-1.54581000	0.33694100	-3.44622900
C	-0.24635000	0.94507000	-3.03732400
C	-0.08046500	2.14055400	-2.37037200
C	-1.21052700	2.97284500	-1.89127000
C	-2.20264600	1.92653400	-1.49034500
F	-4.06100900	-2.76906100	-0.30378200
F	-2.46345500	-4.61982700	-0.46077500
F	-1.63196800	-4.07124900	-2.70240600
F	0.76301500	-4.62476600	-2.19402000
F	1.57773200	-3.24737800	-4.05814200
F	3.56755000	-2.86693700	-2.62139400
F	3.97326500	-0.45548700	-3.48952200
F	5.30487700	0.22999800	-1.50929600
F	4.27464400	2.38946400	-1.92562300
F	4.37117900	3.27995300	0.30204300
F	2.32262300	4.55967300	0.88178500
F	-2.74662000	2.69113700	3.23120900
F	-4.06954800	0.67587900	3.23234200
F	-4.79613700	-0.71095000	1.38104100
F	-2.82140400	-1.25648800	4.10702200
F	-0.94826600	0.15695100	5.03213600
F	3.96800900	2.30009400	2.49794000
F	5.07469600	0.18894900	2.13525200
F	5.08044700	-1.38281300	0.26219900
F	-0.64678600	-4.95419000	1.12389900
F	-1.79872000	-3.72537600	3.07904800
F	0.72082400	-3.67687100	3.57202900
F	0.58382800	-1.77094700	5.06860200
F	2.36269700	-0.08082400	4.68133300
F	3.83387000	-1.67294800	3.22532400
F	-1.79272400	-1.84518400	-4.45589000
F	0.61005700	-1.25077600	-5.01745600
F	1.51604700	4.73884500	-1.55012100
F	-0.83022800	5.14768100	-0.99538300
F	-1.37326900	4.70881000	1.34446700
F	-3.62509900	3.42566300	0.99808000
F	-4.89155000	1.12486900	-0.23854700
F	-4.54784500	-0.58486100	-2.06268600
F	-3.65731800	1.43308500	-3.25263000
F	-1.86456900	0.68208100	-4.72042800
F	-1.69690700	3.75615600	-2.89362300
H	-3.80682900	5.17675100	-0.47590200

O	-3.54220200	4.69392800	-1.26893400
H	-3.12291500	5.35609600	-1.83252800
PC			
C	-2.66045000	-1.45199100	0.98614300
C	-2.78084900	-2.29804000	-0.22443100
C	-1.76014200	-3.47643500	-0.36267400
C	-1.07528300	-3.20351600	-1.81426600
C	0.45764400	-3.32013100	-1.95582900
C	1.22609900	-2.43118600	-3.05048700
C	2.60616900	-1.97295400	-2.27265800
C	3.17683100	-0.53209900	-2.39334000
C	4.01031900	0.16617900	-1.14877400
C	3.45043800	1.65582000	-1.11989400
C	3.31106400	2.45501600	0.22088200
C	1.95178900	3.37257500	0.33524100
C	1.13870200	2.58792100	1.28741500
C	-0.22504200	2.67166000	1.44736700
C	-0.85699900	1.77272500	2.27561500
C	-2.32546200	1.87790500	2.22034800
C	-3.00946700	0.47474100	2.42709900
C	-3.54223300	-0.24689400	1.11381800
C	-1.88679200	-1.66579000	2.03838700
C	-2.07964600	-0.66556600	3.13013900
C	-0.72082000	-0.26329600	3.75728400
C	-0.14036700	0.83060400	2.95979500
C	1.22116100	0.75569000	2.81182500
C	1.85169200	1.61074100	1.93980400
C	3.27969800	1.58655600	1.55716900
C	3.83928800	0.12846000	1.60829800
C	3.95057000	-0.61696900	0.20425000
C	2.79429300	-1.53382400	0.22402500
C	2.21566600	-2.14729500	-0.85890900
C	1.06839100	-2.87888300	-0.69137300
C	0.51637300	-3.02003300	0.55455300
C	-0.79409700	-3.62448200	0.87187900
C	-1.10303500	-2.90989300	2.25132400
C	0.30701500	-2.58226300	2.87541800
C	0.48016600	-1.32849800	3.80459000
C	1.82419500	-0.41573000	3.48173800
C	2.94952300	-0.91665300	2.52762000
C	2.27153100	-1.71116100	1.48144300
C	1.12054100	-2.44114100	1.64599000
C	-2.51416100	-1.38275700	-1.36598600
C	-1.55335900	-1.82735400	-2.16584700

C	-1.16254100	-1.19274800	-3.44840900
C	0.39590900	-1.24941700	-3.67240100
C	0.80769400	0.06147100	-3.11201500
C	2.01238300	0.37406400	-2.51942000
C	2.15013500	1.54712900	-1.81756500
C	1.11139700	2.44719500	-1.76336500
C	1.04646200	3.64504500	-0.89484700
C	-0.58815600	3.85143400	-0.72778800
C	-1.18503800	3.52505300	0.69650200
C	-2.51019200	2.66456400	0.87234100
C	-2.67177200	1.72633400	-0.26418700
C	-3.63733100	0.59355600	-0.18903800
C	-3.36713200	-0.16968300	-1.53720400
C	-2.69198800	0.87471500	-2.48144600
C	-1.54581000	0.33694100	-3.44622900
C	-0.24635000	0.94507000	-3.03732400
C	-0.08046500	2.14055400	-2.37037200
C	-1.21052700	2.97284500	-1.89127000
C	-2.20264600	1.92653400	-1.49034500
F	-4.06100900	-2.76906100	-0.30378200
F	-2.46345500	-4.61982700	-0.46077500
F	-1.63196800	-4.07124900	-2.70240600
F	0.76301500	-4.62476600	-2.19402000
F	1.57773200	-3.24737800	-4.05814200
F	3.56755000	-2.86693700	-2.62139400
F	3.97326500	-0.45548700	-3.48952200
F	5.30487700	0.22999800	-1.50929600
F	4.27464400	2.38946400	-1.92562300
F	4.37117900	3.27995300	0.30204300
F	2.32262300	4.55967300	0.88178500
F	-2.74662000	2.69113700	3.23120900
F	-4.06954800	0.67587900	3.23234200
F	-4.79613700	-0.71095000	1.38104100
F	-2.82140400	-1.25648800	4.10702200
F	-0.94826600	0.15695100	5.03213600
F	3.96800900	2.30009400	2.49794000
F	5.07469600	0.18894900	2.13525200
F	5.08044700	-1.38281300	0.26219900
F	-0.64678600	-4.95419000	1.12389900
F	-1.79872000	-3.72537600	3.07904800
F	0.72082400	-3.67687100	3.57202900
F	0.58382800	-1.77094700	5.06860200
F	2.36269700	-0.08082400	4.68133300
F	3.83387000	-1.67294800	3.22532400

F	-1.79272400	-1.84518400	-4.45589000
F	0.61005700	-1.25077600	-5.01745600
F	1.51604700	4.73884500	-1.55012100
F	-0.83022800	5.14768100	-0.99538300
F	-1.37326900	4.70881000	1.34446700
F	-3.62509900	3.42566300	0.99808000
F	-4.89155000	1.12486900	-0.23854700
F	-4.54784500	-0.58486100	-2.06268600
F	-3.65731800	1.43308500	-3.25263000
F	-1.86456900	0.68208100	-4.72042800
F	-1.69690700	3.75615600	-2.89362300
H	-3.80682900	5.17675100	-0.47590200
O	-3.54220200	4.69392800	-1.26893400
H	-3.12291500	5.35609600	-1.83252800
IP			
C	2.95939500	-1.10043700	-0.87934700
C	3.35132700	-1.41962800	0.52342300
C	2.65059900	-2.66675400	1.16755400
C	2.01964100	-2.07521200	2.55466400
C	0.55978900	-2.43348000	2.92286600
C	-0.32281800	-1.40457500	3.77710600
C	-1.82886000	-1.53683800	3.10225900
C	-2.72002400	-0.29196200	2.82472700
C	-3.78749100	-0.25017200	1.56260300
C	-3.60570000	1.22047000	0.97618200
C	-3.76556400	1.52776100	-0.55010000
C	-2.68584000	2.62396600	-1.14744200
C	-1.77138500	1.74376700	-1.90576600
C	-0.47856200	2.04543100	-2.25814900
C	0.31292900	1.08247300	-2.83689800
C	1.70942100	1.52046000	-3.03177200
C	2.68239400	0.29328200	-2.86367200
C	3.36572500	0.22175600	-1.45433900
C	2.20106100	-1.81587900	-1.69706500
C	2.03996700	-1.19720800	-3.05416400
C	0.58320400	-1.32394000	-3.56420900
C	-0.18948300	-0.16882400	-3.07578400
C	-1.48101700	-0.47346000	-2.72678300
C	-2.25652200	0.47432300	-2.10271600
C	-3.60699400	0.28243900	-1.53237900
C	-3.78906100	-1.18908900	-1.03567100
C	-3.62568200	-1.41800400	0.53430300
C	-2.28083700	-2.01991700	0.64581600
C	-1.50024300	-2.09518800	1.77409900

C	-0.21683100	-2.56922900	1.68010000
C	0.27416500	-2.99896300	0.47661800
C	1.66337400	-3.41063000	0.18981200
C	1.70759200	-3.18147200	-1.37981200
C	0.21549400	-3.36250100	-1.86340500
C	-0.31748300	-2.56753000	-3.10634900
C	-1.81996800	-1.90148100	-2.90210300
C	-2.72526300	-2.27086700	-1.69046800
C	-1.80685500	-2.49190000	-0.55350400
C	-0.52232400	-2.96859800	-0.64251800
C	2.95784700	-0.25311200	1.37713600
C	2.19884000	-0.59417600	2.40785000
C	1.72506000	0.36842300	3.43620400
C	0.23081100	0.06160500	3.84644500
C	-0.50160300	0.93941300	2.90450800
C	-1.79047300	0.79567700	2.45130100
C	-2.25647700	1.60312900	1.44275700
C	-1.46294100	2.60719500	0.94100000
C	-1.78111800	3.47623900	-0.21205100
C	-0.26841500	3.97190300	-0.67029000
C	0.27034300	3.29086200	-1.97788100
C	1.75761400	2.76546500	-2.05008400
C	2.23189100	2.35561000	-0.70248700
C	2.96803800	1.27782500	-0.48199000
C	3.36801000	1.11625000	0.95204500
C	2.68743200	2.30399400	1.71377500
C	1.70141700	1.84352600	2.85371300
C	0.30721000	1.91326800	2.36913000
C	-0.17603100	2.74682400	1.39545800
C	0.61468800	3.72781800	0.63892800
C	2.08023400	3.24138400	0.49924000
F	4.70742500	-1.58078200	0.55679900
F	3.61146800	-3.54539400	1.51183300
F	2.80829500	-2.49738300	3.57901600
F	0.57122600	-3.61938600	3.59256600
F	-0.39515700	-1.87254500	5.03392400
F	-2.51556500	-2.42998100	3.85910200
F	-3.42410900	0.02283500	3.94087700
F	-5.02866500	-0.33297400	2.07231900
F	-4.50939500	2.00872700	1.63145700
F	-4.99957500	2.03083000	-0.72953400
F	-3.38101200	3.44338700	-1.97651200
F	1.86547200	2.00076100	-4.29685500
F	3.65501600	0.42816200	-3.78449900

F	4.72443300	0.26978500	-1.59332800
F	2.83312400	-1.87611700	-3.92613400
F	0.61138800	-1.31876200	-4.92599400
F	-4.51138400	0.47101000	-2.53854000
F	-5.03112000	-1.57722200	-1.37414600
F	-4.53766500	-2.37478500	0.88065000
F	1.79636100	-4.74853500	0.40669200
F	2.50031200	-4.10083300	-1.98148600
F	0.01866500	-4.68898000	-2.10168500
F	-0.38839700	-3.42535000	-4.13773100
F	-2.49719300	-2.11292000	-4.05854300
F	-3.43419000	-3.39111400	-1.97862800
F	2.52842000	0.28997200	4.52440300
F	0.05119800	0.51330600	5.11934900
F	-2.45197800	4.58931800	0.18036700
F	-0.32110100	5.29620000	-0.89312400
F	0.09041600	4.16705800	-3.00525800
F	2.56367000	3.73171900	-2.54670600
F	4.72764200	1.20026600	1.06784600
F	3.66088800	3.02490500	2.30969100
F	1.85966800	2.69522300	3.90737300
F	0.65161400	4.91354600	1.33573400
O	2.91151100	4.32384700	0.27279300
H	2.69425300	5.02463600	0.91145400

C₁-S_N2'-C60-F_b

RC

C	-2.66045000	-1.45199100	0.98614300
C	-2.78084900	-2.29804000	-0.22443100
C	-1.76014200	-3.47643500	-0.36267400
C	-1.07528300	-3.20351600	-1.81426600
C	0.45764400	-3.32013100	-1.95582900
C	1.22609900	-2.43118600	-3.05048700
C	2.60616900	-1.97295400	-2.27265800
C	3.17683100	-0.53209900	-2.39334000
C	4.01031900	0.16617900	-1.14877400
C	3.45043800	1.65582000	-1.11989400
C	3.31106400	2.45501600	0.22088200
C	1.95178900	3.37257500	0.33524100
C	1.13870200	2.58792100	1.28741500
C	-0.22504200	2.67166000	1.44736700
C	-0.85699900	1.77272500	2.27561500
C	-2.32546200	1.87790500	2.22034800
C	-3.00946700	0.47474100	2.42709900
C	-3.54223300	-0.24689400	1.11381800

C	-1.88679200	-1.66579000	2.03838700
C	-2.07964600	-0.66556600	3.13013900
C	-0.72082000	-0.26329600	3.75728400
C	-0.14036700	0.83060400	2.95979500
C	1.22116100	0.75569000	2.81182500
C	1.85169200	1.61074100	1.93980400
C	3.27969800	1.58655600	1.55716900
C	3.83928800	0.12846000	1.60829800
C	3.95057000	-0.61696900	0.20425000
C	2.79429300	-1.53382400	0.22402500
C	2.21566600	-2.14729500	-0.85890900
C	1.06839100	-2.87888300	-0.69137300
C	0.51637300	-3.02003300	0.55455300
C	-0.79409700	-3.62448200	0.87187900
C	-1.10303500	-2.90989300	2.25132400
C	0.30701500	-2.58226300	2.87541800
C	0.48016600	-1.32849800	3.80459000
C	1.82419500	-0.41573000	3.48173800
C	2.94952300	-0.91665300	2.52762000
C	2.27153100	-1.71116100	1.48144300
C	1.12054100	-2.44114100	1.64599000
C	-2.51416100	-1.38275700	-1.36598600
C	-1.55335900	-1.82735400	-2.16584700
C	-1.16254100	-1.19274800	-3.44840900
C	0.39590900	-1.24941700	-3.67240100
C	0.80769400	0.06147100	-3.11201500
C	2.01238300	0.37406400	-2.51942000
C	2.15013500	1.54712900	-1.81756500
C	1.11139700	2.44719500	-1.76336500
C	1.04646200	3.64504500	-0.89484700
C	-0.58815600	3.85143400	-0.72778800
C	-1.18503800	3.52505300	0.69650200
C	-2.51019200	2.66456400	0.87234100
C	-2.67177200	1.72633400	-0.26418700
C	-3.63733100	0.59355600	-0.18903800
C	-3.36713200	-0.16968300	-1.53720400
C	-2.69198800	0.87471500	-2.48144600
C	-1.54581000	0.33694100	-3.44622900
C	-0.24635000	0.94507000	-3.03732400
C	-0.08046500	2.14055400	-2.37037200
C	-1.21052700	2.97284500	-1.89127000
C	-2.20264600	1.92653400	-1.49034500
F	-4.06100900	-2.76906100	-0.30378200
F	-2.46345500	-4.61982700	-0.46077500

F	-1.63196800	-4.07124900	-2.70240600
F	0.76301500	-4.62476600	-2.19402000
F	1.57773200	-3.24737800	-4.05814200
F	3.56755000	-2.86693700	-2.62139400
F	3.97326500	-0.45548700	-3.48952200
F	5.30487700	0.22999800	-1.50929600
F	4.27464400	2.38946400	-1.92562300
F	4.37117900	3.27995300	0.30204300
F	2.32262300	4.55967300	0.88178500
F	-2.74662000	2.69113700	3.23120900
F	-4.06954800	0.67587900	3.23234200
F	-4.79613700	-0.71095000	1.38104100
F	-2.82140400	-1.25648800	4.10702200
F	-0.94826600	0.15695100	5.03213600
F	3.96800900	2.30009400	2.49794000
F	5.07469600	0.18894900	2.13525200
F	5.08044700	-1.38281300	0.26219900
F	-0.64678600	-4.95419000	1.12389900
F	-1.79872000	-3.72537600	3.07904800
F	0.72082400	-3.67687100	3.57202900
F	0.58382800	-1.77094700	5.06860200
F	2.36269700	-0.08082400	4.68133300
F	3.83387000	-1.67294800	3.22532400
F	-1.79272400	-1.84518400	-4.45589000
F	0.61005700	-1.25077600	-5.01745600
F	1.51604700	4.73884500	-1.55012100
F	-0.83022800	5.14768100	-0.99538300
F	-1.37326900	4.70881000	1.34446700
F	-3.62509900	3.42566300	0.99808000
F	-4.89155000	1.12486900	-0.23854700
F	-4.54784500	-0.58486100	-2.06268600
F	-3.65731800	1.43308500	-3.25263000
F	-1.86456900	0.68208100	-4.72042800
F	-1.69690700	3.75615600	-2.89362300
H	-3.80682900	5.17675100	-0.47590200
O	-3.54220200	4.69392800	-1.26893400
H	-3.12291500	5.35609600	-1.83252800
TS	imaginary vibrational frequency		-828.07 cm ⁻¹
C	-2.66045000	-1.45199100	0.98614300
C	-2.78084900	-2.29804000	-0.22443100
C	-1.76014200	-3.47643500	-0.36267400
C	-1.07528300	-3.20351600	-1.81426600
C	0.45764400	-3.32013100	-1.95582900
C	1.22609900	-2.43118600	-3.05048700

C	2.60616900	-1.97295400	-2.27265800
C	3.17683100	-0.53209900	-2.39334000
C	4.01031900	0.16617900	-1.14877400
C	3.45043800	1.65582000	-1.11989400
C	3.31106400	2.45501600	0.22088200
C	1.95178900	3.37257500	0.33524100
C	1.13870200	2.58792100	1.28741500
C	-0.22504200	2.67166000	1.44736700
C	-0.85699900	1.77272500	2.27561500
C	-2.32546200	1.87790500	2.22034800
C	-3.00946700	0.47474100	2.42709900
C	-3.54223300	-0.24689400	1.11381800
C	-1.88679200	-1.66579000	2.03838700
C	-2.07964600	-0.66556600	3.13013900
C	-0.72082000	-0.26329600	3.75728400
C	-0.14036700	0.83060400	2.95979500
C	1.22116100	0.75569000	2.81182500
C	1.85169200	1.61074100	1.93980400
C	3.27969800	1.58655600	1.55716900
C	3.83928800	0.12846000	1.60829800
C	3.95057000	-0.61696900	0.20425000
C	2.79429300	-1.53382400	0.22402500
C	2.21566600	-2.14729500	-0.85890900
C	1.06839100	-2.87888300	-0.69137300
C	0.51637300	-3.02003300	0.55455300
C	-0.79409700	-3.62448200	0.87187900
C	-1.10303500	-2.90989300	2.25132400
C	0.30701500	-2.58226300	2.87541800
C	0.48016600	-1.32849800	3.80459000
C	1.82419500	-0.41573000	3.48173800
C	2.94952300	-0.91665300	2.52762000
C	2.27153100	-1.71116100	1.48144300
C	1.12054100	-2.44114100	1.64599000
C	-2.51416100	-1.38275700	-1.36598600
C	-1.55335900	-1.82735400	-2.16584700
C	-1.16254100	-1.19274800	-3.44840900
C	0.39590900	-1.24941700	-3.67240100
C	0.80769400	0.06147100	-3.11201500
C	2.01238300	0.37406400	-2.51942000
C	2.15013500	1.54712900	-1.81756500
C	1.11139700	2.44719500	-1.76336500
C	1.04646200	3.64504500	-0.89484700
C	-0.58815600	3.85143400	-0.72778800
C	-1.18503800	3.52505300	0.69650200

C	-2.51019200	2.66456400	0.87234100
C	-2.67177200	1.72633400	-0.26418700
C	-3.63733100	0.59355600	-0.18903800
C	-3.36713200	-0.16968300	-1.53720400
C	-2.69198800	0.87471500	-2.48144600
C	-1.54581000	0.33694100	-3.44622900
C	-0.24635000	0.94507000	-3.03732400
C	-0.08046500	2.14055400	-2.37037200
C	-1.21052700	2.97284500	-1.89127000
C	-2.20264600	1.92653400	-1.49034500
F	-4.06100900	-2.76906100	-0.30378200
F	-2.46345500	-4.61982700	-0.46077500
F	-1.63196800	-4.07124900	-2.70240600
F	0.76301500	-4.62476600	-2.19402000
F	1.57773200	-3.24737800	-4.05814200
F	3.56755000	-2.86693700	-2.62139400
F	3.97326500	-0.45548700	-3.48952200
F	5.30487700	0.22999800	-1.50929600
F	4.27464400	2.38946400	-1.92562300
F	4.37117900	3.27995300	0.30204300
F	2.32262300	4.55967300	0.88178500
F	-2.74662000	2.69113700	3.23120900
F	-4.06954800	0.67587900	3.23234200
F	-4.79613700	-0.71095000	1.38104100
F	-2.82140400	-1.25648800	4.10702200
F	-0.94826600	0.15695100	5.03213600
F	3.96800900	2.30009400	2.49794000
F	5.07469600	0.18894900	2.13525200
F	5.08044700	-1.38281300	0.26219900
F	-0.64678600	-4.95419000	1.12389900
F	-1.79872000	-3.72537600	3.07904800
F	0.72082400	-3.67687100	3.57202900
F	0.58382800	-1.77094700	5.06860200
F	2.36269700	-0.08082400	4.68133300
F	3.83387000	-1.67294800	3.22532400
F	-1.79272400	-1.84518400	-4.45589000
F	0.61005700	-1.25077600	-5.01745600
F	1.51604700	4.73884500	-1.55012100
F	-0.83022800	5.14768100	-0.99538300
F	-1.37326900	4.70881000	1.34446700
F	-3.62509900	3.42566300	0.99808000
F	-4.89155000	1.12486900	-0.23854700
F	-4.54784500	-0.58486100	-2.06268600
F	-3.65731800	1.43308500	-3.25263000

F	-1.86456900	0.68208100	-4.72042800
F	-1.69690700	3.75615600	-2.89362300
H	-3.80682900	5.17675100	-0.47590200
O	-3.54220200	4.69392800	-1.26893400
H	-3.12291500	5.35609600	-1.83252800
IP			
C	2.77350900	1.50011300	-0.34820100
C	3.25868100	0.57885200	-1.39919100
C	2.56842500	0.68963700	-2.80032800
C	2.04586000	-0.82647300	-3.07368600
C	0.60847400	-1.03800400	-3.60843200
C	-0.18450100	-2.37878400	-3.23437700
C	-1.73624900	-1.85106000	-2.97719000
C	-2.59411200	-2.36804100	-1.78593700
C	-3.73118100	-1.41542100	-1.04920800
C	-3.51859800	-1.71932800	0.49962000
C	-3.76317400	-0.63434700	1.60253300
C	-2.69116000	-0.66476800	2.86011200
C	-1.89630700	0.56088800	2.61033000
C	-0.63981500	0.81296600	3.10310100
C	0.08286000	1.89791400	2.62261700
C	1.53350600	1.76794100	2.94306300
C	2.47061100	2.41502700	1.86995900
C	3.33507900	1.37298600	1.03444500
C	1.93220800	2.50986200	-0.50064100
C	1.74878400	3.31921300	0.73713800
C	0.27172100	3.75951100	0.92677900
C	-0.46122700	2.71737200	1.67258000
C	-1.73078200	2.47639400	1.19455700
C	-2.42964300	1.37921600	1.63647900
C	-3.72479500	0.88175000	1.11708700
C	-3.92038200	1.26169600	-0.38965700
C	-3.67734600	0.09279600	-1.45131100
C	-2.35395600	0.42535400	-2.01818300
C	-1.51380700	-0.41282300	-2.71332500
C	-0.25654600	0.01851300	-3.05542100
C	0.14389800	1.29014800	-2.74164500
C	1.50386900	1.84725200	-2.89545400
C	1.45083600	3.00074200	-1.81645300
C	-0.06229800	3.42018900	-1.72290800
C	-0.64281000	3.98119700	-0.37561700
C	-2.10805800	3.34669400	0.05965000
C	-2.93932200	2.46969600	-0.92134000
C	-1.96698200	1.71245600	-1.73547300

C	-0.71369300	2.14257000	-2.08745000
C	2.95364800	-0.78489100	-0.88660500
C	2.25564900	-1.50579800	-1.75372400
C	1.90333800	-2.93214700	-1.56043700
C	0.42870600	-3.21192500	-2.05309300
C	-0.32452900	-2.95894600	-0.80496300
C	-1.64069200	-2.58597900	-0.67740900
C	-2.12718700	-2.21019000	0.55000100
C	-1.32526500	-2.28248300	1.65917200
C	-1.68214900	-1.84062600	3.02015100
C	-0.19676900	-1.63438300	3.68076000
C	0.26500000	-0.14984800	3.80844700
C	1.54060000	0.25631300	3.08388300
C	2.28189300	-0.55711200	2.35394700
C	3.43510700	-0.10273400	1.53212800
C	3.53723100	-1.21190300	0.42399200
C	2.85915500	-2.52023100	0.99959400
C	1.90690900	-3.27160200	-0.01877700
C	0.49189000	-2.98524900	0.30153500
C	-0.01230200	-2.65753100	1.52925000
C	0.76750600	-2.52841900	2.76681300
C	2.20898700	-2.05064400	2.43167800
F	4.60936400	0.73361000	-1.53261800
F	3.52610700	0.95364100	-3.70903900
F	2.89630500	-1.40214100	-3.96659200
F	0.64900000	-0.94450400	-4.96621900
F	-0.19743300	-3.16464500	-4.32355700
F	-2.40512800	-2.04455900	-4.14135600
F	-3.21993600	-3.51887900	-2.13856300
F	-4.94322300	-1.88290900	-1.39444700
F	-4.33577700	-2.77183700	0.80143400
F	-4.98869700	-0.86108100	2.11065900
F	-3.41926600	-0.54803000	3.99920600
F	1.80498700	2.33464800	4.15581800
F	3.32658800	3.21907800	2.52901400
F	4.61027100	1.85239000	0.97818900
F	2.48516000	4.45605300	0.58848200
F	0.26928100	4.92127300	1.63549800
F	-4.70909300	1.52660600	1.81183800
F	-5.19271200	1.67372500	-0.53245800
F	-4.60612500	0.26926800	-2.43685300
F	1.63259300	2.43343100	-4.11699000
F	2.20610300	4.06135500	-2.18981000
F	-0.30011900	4.34269400	-2.69611100

F	-0.80644800	5.30593500	-0.53201800
F	-2.87028400	4.38880100	0.48059100
F	-3.69966300	3.27756000	-1.70429100
F	2.78013700	-3.70410000	-2.24595600
F	0.34643600	-4.53034700	-2.38352900
F	-2.28382400	-2.84472300	3.71141000
F	-0.21726000	-2.16893400	4.91353300
F	0.35923200	0.16390100	5.13388400
F	4.55488500	-0.20882300	2.30349000
F	4.85080000	-1.46162000	0.17570300
F	3.85664600	-3.38570700	1.29539400
F	2.13659300	-4.60998600	0.10845900
F	0.88416600	-3.75727800	3.36544000
O	3.07509600	-2.40516700	3.45543700
H	3.10241000	-3.37489000	3.51797900

C₁-S_N2'-C52-F_c

RC

C	2.60262400	-1.63839900	-0.79173800
C	2.77926900	-2.21344300	0.56142600
C	1.76720900	-3.32708400	0.99163000
C	1.15087500	-2.74869900	2.38264800
C	-0.37397000	-2.81828300	2.61457000
C	-1.09049100	-1.71616800	3.53456400
C	-2.50810900	-1.41828400	2.74417200
C	-3.07138600	0.02174900	2.58388900
C	-3.96461400	0.45227700	1.26222500
C	-3.40493300	1.89685700	0.89414100
C	-3.33017700	2.39465500	-0.58907400
C	-1.97577000	3.25290400	-0.95376100
C	-1.21026500	2.26713300	-1.74405700
C	0.14315600	2.29471800	-1.97170900
C	0.74321100	1.24685400	-2.62806500
C	2.21296400	1.36313500	-2.67564900
C	2.88792800	-0.05917700	-2.61596600
C	3.47777200	-0.49591600	-1.20721100
C	1.78587000	-2.06545000	-1.74136700
C	1.92531300	-1.31683200	-3.02582700
C	0.53583200	-1.04463900	-3.65784100
C	-0.00525600	0.19180600	-3.07155000
C	-1.35875100	0.16343900	-2.84949700
C	-1.95301500	1.18551800	-2.14921400
C	-3.36214200	1.26378300	-1.71305800
C	-3.92573900	-0.16504700	-1.43218500
C	-3.97162400	-0.59835200	0.10026500

C	-2.81772400	-1.51063600	0.22078100
C	-2.18678100	-1.88837600	1.38083000
C	-1.04410600	-2.64368900	1.31554800
C	-0.54949200	-3.04521200	0.10307000
C	0.74295000	-3.72045200	-0.13773300
C	0.98896600	-3.31710000	-1.64873100
C	-0.44879400	-3.11359800	-2.26261200
C	-0.66621100	-2.08508500	-3.42718600
C	-1.99475700	-1.11180100	-3.23845300
C	-3.07839500	-1.38953100	-2.15284500
C	-2.35309600	-1.95298800	-0.99414800
C	-1.20641400	-2.70643100	-1.05601200
C	2.56581100	-1.07710100	1.49572500
C	1.64636100	-1.33459000	2.41598800
C	1.31454200	-0.44541800	3.55558600
C	-0.23235000	-0.43956200	3.85461900
C	-0.66932000	0.72392700	3.04526100
C	-1.90083200	0.91971200	2.45859700
C	-2.07107300	1.92181300	1.53409500
C	-1.03635700	2.78274700	1.24674800
C	-1.01006000	3.77615500	0.14648600
C	0.61760800	3.92058100	-0.13341100
C	1.12634200	3.28760000	-1.47865600
C	2.44675700	2.41769200	-1.53030500
C	2.65797400	1.72145700	-0.23615500
C	3.62687500	0.59699200	-0.11434900
C	3.42502200	0.13505300	1.37301100
C	2.79645900	1.35924100	2.10842300
C	1.69548400	1.04574700	3.21462900
C	0.37857100	1.56394300	2.74284700
C	0.18190900	2.59545400	1.84942500
C	1.28771500	3.30045700	1.16045000
C	2.26243000	2.18623500	0.94386800
F	4.06189700	-2.67211500	0.67616300
F	2.47519300	-4.43060400	1.29627700
F	1.74990200	-3.41211200	3.40882500
F	-0.66800700	-4.04298800	3.13106800
F	-1.39323100	-2.29996600	4.70662500
F	-3.44863500	-2.20920400	3.32174600
F	-3.81084600	0.33864100	3.67739500
F	-5.23955700	0.60624000	1.66293000
F	-4.18743000	2.79445300	1.56423700
F	-4.39262100	3.19482700	-0.79230500
F	-2.37051600	4.29459100	-1.73043800

F	2.57950200	1.93970000	-3.85532500
F	3.91015800	-0.04197800	-3.49145300
F	4.72095600	-1.01416500	-1.42253100
F	2.62238800	-2.09983200	-3.89297800
F	0.70213400	-0.89808600	-5.00096800
F	-4.08816400	1.77265700	-2.75237600
F	-5.18421500	-0.20379800	-1.90272700
F	-5.10525100	-1.34554800	0.25340300
F	0.57527600	-5.07110600	-0.09570000
F	1.64134600	-4.29678800	-2.31896100
F	-0.88922400	-4.32901100	-2.69037700
F	-0.82948900	-2.78202600	-4.56297900
F	-2.58571700	-1.02357200	-4.45652500
F	-3.99396500	-2.26559700	-2.63738800
F	1.99005600	-0.88357800	4.64689300
F	-0.38663700	-0.15339000	5.17715900
F	-1.44302500	4.98810000	0.57712800
F	0.91240400	5.23047800	-0.15810300
F	1.25230700	4.29391000	-2.38672600
F	3.52501100	3.17568700	-1.84115600
F	4.88644600	1.11977100	-0.22333800
F	4.62990800	-0.17370800	1.91875900
F	3.80003700	2.05595100	2.70602600
F	2.07333700	1.65075800	4.37046200
F	1.81335200	4.27910900	1.94628700
H	4.37895300	4.35733400	1.57168500
O	4.18615200	4.24906400	0.63178000
H	4.97534300	3.82509800	0.26988700
TS	imaginary vibrational frequency		-886.93 cm ⁻¹
C	2.72686600	0.45324200	1.49872900
C	2.85934400	1.86884100	1.08374400
C	1.89190100	2.90108100	1.75244400
C	1.15566600	3.59312700	0.47744800
C	-0.37321600	3.80630100	0.50915200
C	-1.22109200	3.79746400	-0.86092100
C	-2.58537800	2.97859900	-0.46891900
C	-3.22895200	1.94229400	-1.43299000
C	-4.05107200	0.64249200	-0.84625300
C	-3.57243900	-0.55303000	-1.78575100
C	-3.42255700	-2.00442700	-1.21237800
C	-2.10057100	-2.79923300	-1.74515200
C	-1.22654700	-2.75469500	-0.55722200
C	0.13387200	-2.93494200	-0.54292600
C	0.83072700	-2.74744900	0.61760100

C	2.28438200	-2.88810600	0.45195000
C	3.04520700	-1.94678200	1.43267600
C	3.56889500	-0.59156000	0.81642600
C	2.02041000	-0.00721400	2.52037700
C	2.19379300	-1.47286600	2.74819500
C	0.82524200	-2.13548500	3.05577700
C	0.17446900	-2.45103700	1.77703100
C	-1.18684700	-2.29222900	1.77645400
C	-1.87993300	-2.40001700	0.59447000
C	-3.31853200	-2.14534200	0.37669000
C	-3.81649800	-1.03115900	1.34380200
C	-3.91994400	0.41905200	0.70136300
C	-2.72173500	1.09628700	1.22935200
C	-2.14407700	2.23234800	0.72532200
C	-0.96521300	2.68659700	1.25683000
C	-0.37669000	2.01961500	2.29916300
C	0.96792900	2.27520500	2.85722700
C	1.28922900	0.86009000	3.48742600
C	-0.12047700	0.24323900	3.84577800
C	-0.32465200	-1.31071400	3.81560800
C	-1.72234200	-1.80072500	3.06178000
C	-2.85608600	-0.79990400	2.67626000
C	-2.16780700	0.45657700	2.31107400
C	-0.97871500	0.90501000	2.83455700
C	2.52236700	1.85731800	-0.35620400
C	1.54859200	2.70834500	-0.66316000
C	1.08134500	3.01810600	-2.03678300
C	-0.46720000	3.24804900	-2.12384500
C	-0.93879700	1.89770000	-2.53763600
C	-2.13256200	1.29540800	-2.18966200
C	-2.30549900	-0.05439000	-2.38280100
C	-1.31612400	-0.80719600	-2.99176000
C	-1.25182700	-2.29522100	-2.94286700
C	0.37874400	-2.56956700	-2.94618300
C	1.00786500	-3.23302000	-1.69038700
C	2.44824300	-2.78861700	-1.12018100
C	2.90916100	-1.42133600	-1.65714300
C	3.73184800	-0.44451000	-0.75887400
C	3.30877900	1.00855000	-1.29716700
C	2.45090800	0.74991400	-2.53648100
C	1.39593200	1.82725600	-3.00329400
C	0.06476400	1.15590700	-3.11681300
C	-0.12002300	-0.20271000	-3.34127300
C	0.97650900	-1.15502000	-3.12131700

C	1.85063500	-0.58657500	-2.18140200
F	4.15959100	2.25628500	1.25715700
F	2.64603500	3.84662200	2.34516000
F	1.73452900	4.80946500	0.28061000
F	-0.62838000	4.98227500	1.14558300
F	-1.57027200	5.06919900	-1.12370200
F	-3.52038900	3.90701700	-0.13349900
F	-4.07361700	2.59171500	-2.27639100
F	-5.35926900	0.84135900	-1.09539000
F	-4.48534000	-0.63183400	-2.79965000
F	-4.50846300	-2.69800000	-1.60144900
F	-2.48183000	-4.07953100	-2.00116800
F	2.61393400	-4.16880500	0.79910700
F	4.11974400	-2.63213200	1.87077800
F	4.82316400	-0.40043400	1.32527800
F	2.99656500	-1.65892500	3.82946900
F	1.05318400	-3.27531800	3.76434500
F	-3.99525600	-3.28492400	0.70940500
F	-5.04153100	-1.37841700	1.77461700
F	-5.00778700	1.01740400	1.27337200
F	0.88353800	3.16709100	3.88302400
F	2.02980100	0.99484900	4.61448500
F	-0.45789400	0.68223600	5.09038100
F	-0.37066500	-1.74602500	5.08489000
F	-2.23479800	-2.80684700	3.81325800
F	-3.68990100	-0.62527400	3.73149900
F	1.72612700	4.14554300	-2.43868900
F	-0.68550800	4.11936000	-3.14993100
F	-1.75106000	-2.83653800	-4.08259900
F	0.62625400	-3.36662000	-4.00196600
F	1.06198300	-4.57815000	-1.89619500
F	3.37181700	-3.72964100	-1.48205900
F	5.04580600	-0.62640500	-1.02184500
F	4.44337500	1.69990000	-1.58720300
F	3.34334500	0.65188300	-3.58915800
F	1.78182800	2.36023400	-4.19114000
F	2.02578600	-1.45022300	-4.48309000
H	4.20900500	-2.63315300	-2.79396300
O	3.76652300	-1.76450200	-2.88634100
H	3.05748700	-1.67998300	-3.77271900
IP			
C	2.85429800	0.03869300	1.26337100
C	2.98584700	1.51058700	1.20860400
C	2.10129000	2.34063000	2.19733400

C	1.28545500	3.33922800	1.20688700
C	-0.23035500	3.54252900	1.42105900
C	-1.17953400	3.89468100	0.17092100
C	-2.53474400	3.00350500	0.45014000
C	-3.28318600	2.25332500	-0.68940600
C	-4.08490600	0.84243500	-0.38931100
C	-3.71176000	-0.07398400	-1.64073000
C	-3.53505500	-1.62702900	-1.47636400
C	-2.27427400	-2.26696100	-2.30375700
C	-1.30428000	-2.52318400	-1.22020200
C	0.05341400	-2.69354500	-1.36373300
C	0.84074200	-2.79124100	-0.25143700
C	2.27336200	-2.91563000	-0.55880900
C	3.12319800	-2.26601800	0.57179900
C	3.62982900	-0.79905400	0.28800300
C	2.21038000	-0.66414800	2.18069600
C	2.37988800	-2.13758400	2.02522200
C	1.02711200	-2.85331200	2.25752500
C	0.27885400	-2.81003300	0.99436100
C	-1.07381400	-2.66050300	1.14431600
C	-1.85744100	-2.46426200	0.03249900
C	-3.30457200	-2.16933900	0.00716100
C	-3.70687700	-1.34314600	1.26568500
C	-3.83666300	0.22553900	1.03283000
C	-2.58674300	0.74774300	1.61877700
C	-2.02044600	1.97297000	1.37435800
C	-0.79108500	2.26975000	1.90303900
C	-0.13793900	1.35560900	2.68727800
C	1.25256200	1.45462700	3.17968500
C	1.58480000	-0.07710700	3.39514900
C	0.19629500	-0.75853500	3.70093600
C	-0.04203300	-2.25248700	3.29382900
C	-1.50113600	-2.52661800	2.55137800
C	-2.64155800	-1.46188600	2.53157400
C	-1.96109400	-0.15187500	2.44794800
C	-0.72225000	0.14226200	2.96461900
C	2.53243700	1.86399300	-0.15744600
C	1.56730000	2.77764300	-0.15300000
C	1.01243900	3.43522400	-1.36008100
C	-0.54002100	3.68973900	-1.25004200
C	-1.08185000	2.48763500	-1.93874500
C	-2.26611000	1.82236600	-1.67465900
C	-2.49004800	0.56366400	-2.19234300
C	-1.55862800	-0.02640400	-3.02288900

C	-1.50281800	-1.47281400	-3.38819500
C	0.13652900	-1.71043200	-3.56871900
C	0.83464000	-2.70209600	-2.61794500
C	2.34261200	-2.44596300	-2.07793700
C	2.91869800	-1.00898400	-2.37253300
C	3.69221800	-0.24666600	-1.19840600
C	3.24874100	1.29179800	-1.33753200
C	2.36190600	1.39965800	-2.59956500
C	1.21901200	2.51952200	-2.61603100
C	-0.12851500	1.89146200	-2.72749700
C	-0.36054500	0.63065600	-3.23191500
C	0.69795100	-0.33721300	-3.32111700
C	1.87338700	-0.02553500	-2.77850700
F	4.30189500	1.84249000	1.36628000
F	2.92186600	3.09943300	2.94740000
F	1.87934800	4.56146700	1.27986100
F	-0.40145200	4.51582500	2.35669100
F	-1.51816200	5.19069400	0.27616100
F	-3.41150700	3.82080300	1.09092700
F	-4.18202100	3.09889900	-1.25776200
F	-5.40253800	1.10220300	-0.47067700
F	-4.70864800	0.10441600	-2.55688000
F	-4.66096200	-2.20224700	-1.93756900
F	-2.70901300	-3.43536400	-2.84405300
F	2.56771600	-4.25269000	-0.54294400
F	4.21107600	-3.04334800	0.74247800
F	4.91375000	-0.75419900	0.75589900
F	3.25324700	-2.56946300	2.97350900
F	1.27526300	-4.14255500	2.61666900
F	-3.97051800	-3.35961100	0.09123300
F	-4.90118600	-1.79501200	1.68583300
F	-4.86726700	0.64675500	1.82527100
F	1.27305300	2.05418800	4.40198100
F	2.42613300	-0.25832900	4.44207700
F	-0.03247700	-0.64788900	5.03902000
F	0.00000800	-2.99818800	4.40937700
F	-1.97646200	-3.69485900	3.04940100
F	-3.38619100	-1.56820700	3.66006500
F	1.64994200	4.62243000	-1.51703000
F	-0.81638100	4.79420700	-1.99777800
F	-2.07483400	-1.69661600	-4.59573000
F	0.34964500	-2.07905600	-4.85337900
F	0.80489400	-3.94012500	-3.18110600
F	3.16149300	-3.32208400	-2.70709600

F	5.00587700	-0.30318300	-1.53349100
F	4.36846000	2.04943700	-1.48776400
F	3.18911000	1.67673500	-3.64690400
F	1.44993100	3.33511900	-3.67910600
O	3.75371500	-1.08815400	-3.48367800
H	4.53300200	-1.62678900	-3.26714500

C₁-S_N2'-C52-F_d

RC

C	2.60262400	-1.63839900	-0.79173800
C	2.77926900	-2.21344300	0.56142600
C	1.76720900	-3.32708400	0.99163000
C	1.15087500	-2.74869900	2.38264800
C	-0.37397000	-2.81828300	2.61457000
C	-1.09049100	-1.71616800	3.53456400
C	-2.50810900	-1.41828400	2.74417200
C	-3.07138600	0.02174900	2.58388900
C	-3.96461400	0.45227700	1.26222500
C	-3.40493300	1.89685700	0.89414100
C	-3.33017700	2.39465500	-0.58907400
C	-1.97577000	3.25290400	-0.95376100
C	-1.21026500	2.26713300	-1.74405700
C	0.14315600	2.29471800	-1.97170900
C	0.74321100	1.24685400	-2.62806500
C	2.21296400	1.36313500	-2.67564900
C	2.88792800	-0.05917700	-2.61596600
C	3.47777200	-0.49591600	-1.20721100
C	1.78587000	-2.06545000	-1.74136700
C	1.92531300	-1.31683200	-3.02582700
C	0.53583200	-1.04463900	-3.65784100
C	-0.00525600	0.19180600	-3.07155000
C	-1.35875100	0.16343900	-2.84949700
C	-1.95301500	1.18551800	-2.14921400
C	-3.36214200	1.26378300	-1.71305800
C	-3.92573900	-0.16504700	-1.43218500
C	-3.97162400	-0.59835200	0.10026500
C	-2.81772400	-1.51063600	0.22078100
C	-2.18678100	-1.88837600	1.38083000
C	-1.04410600	-2.64368900	1.31554800
C	-0.54949200	-3.04521200	0.10307000
C	0.74295000	-3.72045200	-0.13773300
C	0.98896600	-3.31710000	-1.64873100
C	-0.44879400	-3.11359800	-2.26261200
C	-0.66621100	-2.08508500	-3.42718600
C	-1.99475700	-1.11180100	-3.23845300

C	-3.07839500	-1.38953100	-2.15284500
C	-2.35309600	-1.95298800	-0.99414800
C	-1.20641400	-2.70643100	-1.05601200
C	2.56581100	-1.07710100	1.49572500
C	1.64636100	-1.33459000	2.41598800
C	1.31454200	-0.44541800	3.55558600
C	-0.23235000	-0.43956200	3.85461900
C	-0.66932000	0.72392700	3.04526100
C	-1.90083200	0.91971200	2.45859700
C	-2.07107300	1.92181300	1.53409500
C	-1.03635700	2.78274700	1.24674800
C	-1.01006000	3.77615500	0.14648600
C	0.61760800	3.92058100	-0.13341100
C	1.12634200	3.28760000	-1.47865600
C	2.44675700	2.41769200	-1.53030500
C	2.65797400	1.72145700	-0.23615500
C	3.62687500	0.59699200	-0.11434900
C	3.42502200	0.13505300	1.37301100
C	2.79645900	1.35924100	2.10842300
C	1.69548400	1.04574700	3.21462900
C	0.37857100	1.56394300	2.74284700
C	0.18190900	2.59545400	1.84942500
C	1.28771500	3.30045700	1.16045000
C	2.26243000	2.18623500	0.94386800
F	4.06189700	-2.67211500	0.67616300
F	2.47519300	-4.43060400	1.29627700
F	1.74990200	-3.41211200	3.40882500
F	-0.66800700	-4.04298800	3.13106800
F	-1.39323100	-2.29996600	4.70662500
F	-3.44863500	-2.20920400	3.32174600
F	-3.81084600	0.33864100	3.67739500
F	-5.23955700	0.60624000	1.66293000
F	-4.18743000	2.79445300	1.56423700
F	-4.39262100	3.19482700	-0.79230500
F	-2.37051600	4.29459100	-1.73043800
F	2.57950200	1.93970000	-3.85532500
F	3.91015800	-0.04197800	-3.49145300
F	4.72095600	-1.01416500	-1.42253100
F	2.62238800	-2.09983200	-3.89297800
F	0.70213400	-0.89808600	-5.00096800
F	-4.08816400	1.77265700	-2.75237600
F	-5.18421500	-0.20379800	-1.90272700
F	-5.10525100	-1.34554800	0.25340300
F	0.57527600	-5.07110600	-0.09570000

F	1.64134600	-4.29678800	-2.31896100
F	-0.88922400	-4.32901100	-2.69037700
F	-0.82948900	-2.78202600	-4.56297900
F	-2.58571700	-1.02357200	-4.45652500
F	-3.99396500	-2.26559700	-2.63738800
F	1.99005600	-0.88357800	4.64689300
F	-0.38663700	-0.15339000	5.17715900
F	-1.44302500	4.98810000	0.57712800
F	0.91240400	5.23047800	-0.15810300
F	1.25230700	4.29391000	-2.38672600
F	3.52501100	3.17568700	-1.84115600
F	4.88644600	1.11977100	-0.22333800
F	4.62990800	-0.17370800	1.91875900
F	3.80003700	2.05595100	2.70602600
F	2.07333700	1.65075800	4.37046200
F	1.81335200	4.27910900	1.94628700
H	4.37895300	4.35733400	1.57168500
O	4.18615200	4.24906400	0.63178000
H	4.97534300	3.82509800	0.26988700
TS	imaginary vibrational frequency		-796.22 cm ⁻¹
C	2.73322600	0.44525600	1.49900400
C	2.90160700	1.84875300	1.05111400
C	1.94765500	2.91247300	1.68647600
C	1.22947400	3.58951500	0.38890800
C	-0.29687000	3.81890100	0.41294400
C	-1.13752000	3.79093900	-0.95773300
C	-2.52495900	3.01624800	-0.53980600
C	-3.19862400	1.97130400	-1.47256400
C	-4.05055100	0.70331900	-0.84849200
C	-3.60100900	-0.52686500	-1.75558000
C	-3.47211700	-1.97140200	-1.15560600
C	-2.16503000	-2.81040100	-1.67683400
C	-1.27772100	-2.74032900	-0.49958200
C	0.08336700	-2.93094100	-0.49274700
C	0.78482700	-2.73195600	0.66422500
C	2.23530700	-2.91180200	0.50363200
C	3.00683900	-1.96752000	1.47953800
C	3.55467500	-0.63218600	0.85109800
C	2.02019100	0.01802900	2.52931300
C	2.16572700	-1.44810700	2.78406500
C	0.78677000	-2.07773700	3.09798000
C	0.13514800	-2.40305300	1.82121900
C	-1.22292500	-2.22159300	1.82203600
C	-1.92089600	-2.34672100	0.64566800

C	-3.35719800	-2.07574300	0.43276000
C	-3.83319200	-0.92883400	1.37413800
C	-3.91605500	0.51097900	0.70190600
C	-2.70316000	1.17960300	1.20853800
C	-2.10027900	2.28894600	0.67302100
C	-0.90867800	2.72834500	1.18859800
C	-0.33494500	2.07784200	2.24884700
C	1.01102900	2.32586000	2.80511100
C	1.30413800	0.92032300	3.47356000
C	-0.11576000	0.33492000	3.83965000
C	-0.34595600	-1.21660900	3.84123800
C	-1.74945500	-1.69680200	3.09814400
C	-2.86615100	-0.68378000	2.69642700
C	-2.15779500	0.55279600	2.30212700
C	-0.95859300	0.98896300	2.81137100
C	2.57784700	1.81916900	-0.39279400
C	1.62292300	2.67821100	-0.73402100
C	1.15721000	2.92237100	-2.12606500
C	-0.39366300	3.18914000	-2.20659200
C	-0.90579900	1.84243400	-2.57226800
C	-2.11632500	1.28018700	-2.20834800
C	-2.32448500	-0.07050100	-2.35684100
C	-1.35294300	-0.86678900	-2.93286600
C	-1.31497400	-2.35357300	-2.88795700
C	0.31413600	-2.65623100	-2.92033900
C	0.94981700	-3.27620800	-1.63855200
C	2.41452000	-2.85915200	-1.07934200
C	2.89294000	-1.50337300	-1.61338600
C	3.70543400	-0.52053400	-0.71263000
C	3.31815000	0.90453900	-1.31149100
C	2.38108100	0.58251800	-2.45781800
C	1.43659900	1.66730300	-3.05068800
C	0.07308500	1.05289400	-3.12864000
C	-0.15794400	-0.29889200	-3.29889600
C	0.95690700	-1.27161400	-3.25743300
C	1.85146400	-0.69619600	-2.20717300
F	4.20731600	2.21219700	1.23807900
F	2.71370800	3.86000200	2.25989000
F	1.82010700	4.79801400	0.18111700
F	-0.53715600	5.01339900	1.02109400
F	-1.45692700	5.06218800	-1.25762900
F	-3.42961100	3.98083900	-0.22409000
F	-4.03246300	2.61694700	-2.32961000
F	-5.35443800	0.92817700	-1.09738200

F	-4.51548500	-0.61094900	-2.76814600
F	-4.57380400	-2.65273900	-1.52089200
F	-2.57696500	-4.08993200	-1.88435300
F	2.53690700	-4.19092400	0.87979500
F	4.06803100	-2.66415200	1.93239900
F	4.81193600	-0.45579700	1.35887500
F	2.96460200	-1.62627800	3.86940400
F	0.99114300	-3.20858300	3.82801600
F	-4.04809800	-3.19584400	0.80117000
F	-5.06288000	-1.24598000	1.81609100
F	-4.99067100	1.13765700	1.26826600
F	0.93871300	3.24384800	3.80828000
F	2.04428600	1.06721400	4.59916700
F	-0.45080500	0.80558600	5.07324500
F	-0.39753800	-1.62398200	5.11985700
F	-2.27924300	-2.67957100	3.86846700
F	-3.69200300	-0.47226800	3.75156800
F	1.82726000	4.00213700	-2.60374300
F	-0.59416200	4.03660400	-3.25590900
F	-1.84032700	-2.88892600	-4.02018600
F	0.53793800	-3.50642400	-3.94149200
F	0.97390600	-4.63006800	-1.79304800
F	3.31541900	-3.81087500	-1.41898800
F	5.03137900	-0.72819000	-0.96796800
F	4.45385000	1.55275700	-1.67905200
F	3.57531000	0.35161400	-3.67983800
F	1.87956300	2.11511700	-4.24787700
F	1.60702300	-1.38213400	-4.46914700
H	3.85540600	-0.86949700	-3.35952900
O	3.82662600	-1.83665300	-2.80108600
H	4.71607500	-2.12322100	-2.50808100
IP			
C	2.98365400	0.61621900	0.91085000
C	3.08940300	1.94482000	0.25679900
C	2.22449100	3.10111500	0.86881200
C	1.31200400	3.58861500	-0.39193500
C	-0.19768000	3.84134400	-0.17436600
C	-1.24169400	3.62608000	-1.38018700
C	-2.54507600	2.94660500	-0.64747600
C	-3.34772900	1.78636800	-1.30123400
C	-4.09017200	0.64333200	-0.37612200
C	-3.78148600	-0.71705100	-1.14939400
C	-3.56188200	-2.05763900	-0.36823600
C	-2.34240600	-2.98434200	-0.95454000

C	-1.28637100	-2.72767900	0.04206200
C	0.06155600	-2.90665800	-0.14411100
C	0.92875600	-2.55985300	0.85149400
C	2.33465700	-2.82864800	0.52642700
C	3.25281900	-1.77628600	1.21968300
C	3.70093500	-0.56636300	0.31638100
C	2.41774900	0.35590000	2.07945200
C	2.61270200	-1.05099900	2.53761600
C	1.30357700	-1.60410600	3.14816900
C	0.46244100	-2.07489100	2.04014600
C	-0.87903200	-1.88400400	2.22823600
C	-1.74927400	-2.17027700	1.20449200
C	-3.20337300	-1.92481000	1.18094300
C	-3.53455000	-0.64388600	2.00601700
C	-3.72205400	0.68162700	1.14812200
C	-2.44830500	1.39712400	1.36264700
C	-1.93668800	2.40183800	0.58178700
C	-0.68068000	2.88876200	0.83806300
C	0.05086300	2.39160300	1.88371800
C	1.46666100	2.69449300	2.18675700
C	1.86292400	1.39197000	2.99029600
C	0.52083500	0.89990600	3.66206700
C	0.29712900	-0.62926500	3.92903400
C	-1.20441800	-1.18407600	3.48632500
C	-2.37590000	-0.22273800	3.11875600
C	-1.74100700	0.93148200	2.44478800
C	-0.47736600	1.41302400	2.69408400
C	2.56459500	1.71833100	-1.10647800
C	1.54262800	2.51772500	-1.41008500
C	0.84966300	2.55062100	-2.72872700
C	-0.69520600	2.83041900	-2.61894400
C	-1.25391100	1.45259500	-2.70363800
C	-2.38975000	0.97093300	-2.08230200
C	-2.61135100	-0.38254600	-1.99800700
C	-1.73144600	-1.27354100	-2.58995400
C	-1.69158400	-2.73867900	-2.34103100
C	-0.08298800	-3.08213300	-2.59137900
C	0.73890500	-3.48121900	-1.32219100
C	2.27559100	-3.04618100	-1.04704200
C	2.76903200	-1.86758000	-1.93982200
C	3.62587600	-0.69802600	-1.25846800
C	3.09442100	0.61698800	-1.97717400
C	1.91196100	0.16870300	-2.75752600
C	0.98944600	1.15152900	-3.44472000

C	-0.37379600	0.57011900	-3.28361800
C	-0.61144100	-0.79104100	-3.21967200
C	0.48609700	-1.79609900	-3.29713600
C	1.65629400	-1.13199100	-2.61729100
F	4.40544300	2.30807100	0.20526300
F	3.05561800	4.11399700	1.17898100
F	1.85287000	4.74247800	-0.87107900
F	-0.35119900	5.11642700	0.27828700
F	-1.60915200	4.84303100	-1.81614500
F	-3.39930100	3.96102700	-0.35085000
F	-4.30216400	2.31283400	-2.11139100
F	-5.41656000	0.85596500	-0.45947900
F	-4.83701000	-0.92903800	-1.99132200
F	-4.70304400	-2.76419700	-0.45574700
F	-2.76292000	-4.27457100	-0.88533200
F	2.64955200	-4.03766700	1.08570900
F	4.36590200	-2.42516700	1.61446400
F	5.01846200	-0.34804800	0.60905500
F	3.56390400	-1.05075600	3.50985000
F	1.61564100	-2.63658800	3.97827400
F	-3.81485100	-2.96978500	1.81198700
F	-4.68060000	-0.87018500	2.67094800
F	-4.70413000	1.40154100	1.76796900
F	1.53885700	3.74460000	3.05055700
F	2.78487100	1.66001100	3.94710000
F	0.38907700	1.55334900	4.84908600
F	0.44350200	-0.84630300	5.24503500
F	-1.60344200	-2.04217500	4.45736300
F	-3.03455400	0.14873600	4.24340500
F	1.43020900	3.52352000	-3.47644600
F	-1.05322300	3.51428800	-3.74285400
F	-2.38720400	-3.41841800	-3.28598900
F	-0.02442800	-4.10405500	-3.46361300
F	0.69419600	-4.84077400	-1.22704200
F	3.07250600	-4.11299800	-1.31591200
F	4.90216500	-0.89197000	-1.66382000
F	4.07544100	1.13631500	-2.77090100
F	1.37156000	1.33795400	-4.73675500
F	0.83924300	-2.10219700	-4.57845200
O	3.47661700	-2.39563100	-3.01678500
H	4.12562900	-3.04372300	-2.69488400
C ₁ -S _N 2'-C40-F _g			
RC			
C	-2.73712900	-1.13255400	-0.97542200

C	-3.36129800	0.20855100	-1.10044000
C	-2.84633700	1.11570700	-2.26808400
C	-2.35049000	2.46450800	-1.50630500
C	-0.99404200	3.09088400	-1.89733100
C	-0.15510700	3.91687700	-0.80939000
C	1.40502000	3.48122900	-1.11922600
C	2.41337500	3.17896800	0.02274300
C	3.62863200	2.07814400	-0.17589800
C	3.63555000	1.28351400	1.20335300
C	4.00438600	-0.23702000	1.26757900
C	3.08808200	-1.11254800	2.31136300
C	2.21844400	-1.86136000	1.38034300
C	1.01167200	-2.43652000	1.69170700
C	0.24341600	-2.99525700	0.69828400
C	-1.08088900	-3.44174600	1.17792200
C	-2.16659900	-3.26349600	0.04848000
C	-3.11756300	-1.99877100	0.18636400
C	-1.93678700	-1.72565400	-1.84615500
C	-1.59302400	-3.13107300	-1.47650500
C	-0.09903300	-3.42490700	-1.76313400
C	0.68838600	-2.99607000	-0.59528100
C	1.89652800	-2.42619900	-0.91112300
C	2.64158000	-1.82346500	0.07434400
C	3.89100000	-1.05340500	-0.09795400
C	3.90810000	-0.34288300	-1.48726800
C	3.52378000	1.20383800	-1.47250000
C	2.13942900	1.20302000	-1.98442900
C	1.21481600	2.20831800	-1.84512100
C	-0.07448200	2.00343200	-2.26100700
C	-0.43470900	0.81986900	-2.84724900
C	-1.80443300	0.39822700	-3.20824600
C	-1.61904600	-1.17368900	-3.18850100
C	-0.10304000	-1.41902800	-3.54584700
C	0.64466600	-2.67383400	-2.97240900
C	2.15397400	-2.35426800	-2.36439800
C	2.86737700	-0.98815700	-2.59905700
C	1.79513900	0.02961800	-2.61026700
C	0.50195000	-0.17041300	-3.02776000
C	-3.00881900	0.92034200	0.15878900
C	-2.37472400	2.06580900	-0.06240600
C	-1.99529200	3.04148300	0.98810000
C	-0.61025900	3.72543800	0.68065900
C	0.31755800	2.84160800	1.42806600
C	1.63389100	2.56959400	1.12467200

C	2.28386100	1.53506900	1.75318800
C	1.64956900	0.82098400	2.74405600
C	2.14954300	-0.43577200	3.35040500
C	0.74194800	-1.15981100	3.82057500
C	0.31942400	-2.42914400	2.99887900
C	-1.17695000	-2.63683700	2.52854300
C	-1.84947800	-1.33219300	2.30145700
C	-3.12777600	-1.23976200	1.53887200
C	-3.37958300	0.31650200	1.47458300
C	-2.52897000	0.92101700	2.63961000
C	-1.81514500	2.31644900	2.37448600
C	-0.33469400	2.11229400	2.39777300
C	0.34591900	1.11445000	3.06670800
C	-0.33128200	0.00824200	3.78541700
C	-1.54258800	-0.20603300	2.93312300
F	-4.71041300	0.02029800	-1.21688700
F	-3.91078800	1.45210900	-3.02489400
F	-3.29048000	3.43176000	-1.70260100
F	-1.19247300	3.90427700	-2.97212200
F	-0.28119400	5.22214000	-1.10343400
F	1.92273800	4.43323000	-1.93772000
F	2.99679300	4.33673100	0.42668400
F	4.78560800	2.75978500	-0.25435500
F	4.52260000	1.93047700	2.01730000
F	5.28435900	-0.31720100	1.67413600
F	3.93107700	-1.95362900	2.96567700
F	-1.02313300	-4.76693100	1.48926800
F	-2.94513700	-4.36084500	0.08360300
F	-4.39368500	-2.42438000	-0.03869400
F	-2.33075000	-3.96227800	-2.26186500
F	0.04213900	-4.76412900	-1.96110300
F	4.92646600	-1.94473000	-0.10043400
F	5.15419400	-0.44703000	-1.98094700
F	4.31275000	1.80251400	-2.41305000
F	-2.08145000	0.75965300	-4.49164200
F	-2.41620000	-1.77394200	-4.10533600
F	0.00524800	-1.45141600	-4.90318900
F	0.78911700	-3.55627900	-3.97404400
F	2.95941100	-3.36391400	-2.77884100
F	3.53223500	-1.02108400	-3.78089800
F	-2.95678300	3.99143700	1.05656300
F	-0.62762100	4.95435500	1.26987500
F	2.85677800	-0.17968100	4.48039700
F	0.89081100	-1.53493000	5.10311000

F	0.67990900	-3.52956700	3.71551900
F	-1.87671600	-3.34398000	3.44957700
F	-4.10384500	-1.79726600	2.31122000
F	-4.69654200	0.54994500	1.69536800
F	-3.33896300	1.06339600	3.71910200
F	-2.19946400	3.18219100	3.34704100
F	-0.70477500	0.33745700	5.05256400
H	-5.52376000	2.92000700	-1.04286500
O	-5.42703500	2.53118500	-0.16432400
H	-6.11104200	1.85094400	-0.12746900
TS	imaginary vibrational frequency		-792.44 cm ⁻¹
C	-2.76205800	-0.93008700	-0.95625600
C	-3.38362300	0.39492600	-1.19342400
C	-2.71122400	1.22786100	-2.33689400
C	-2.03886900	2.38954500	-1.50950500
C	-0.78943900	3.09912900	-2.00219600
C	0.10728800	3.88966100	-0.93384600
C	1.63847900	3.35636400	-1.21088900
C	2.60808400	3.01924900	-0.04175100
C	3.75004900	1.84199700	-0.18809400
C	3.69443300	1.09200800	1.21783400
C	3.95697500	-0.44640200	1.33440300
C	2.97141900	-1.22834900	2.39210800
C	2.06743300	-1.95108400	1.47334700
C	0.82442400	-2.44583100	1.78423700
C	0.03470400	-2.97860000	0.79336800
C	-1.32783800	-3.30909600	1.25937300
C	-2.37887700	-3.08597000	0.10841400
C	-3.23499800	-1.75438300	0.19391900
C	-2.00696900	-1.60741800	-1.80929600
C	-1.77535300	-3.02763500	-1.40418800
C	-0.30565100	-3.44146000	-1.66263200
C	0.49467600	-3.04168600	-0.49381500
C	1.73713700	-2.55222500	-0.80696800
C	2.50679600	-1.97377800	0.17279200
C	3.80512800	-1.29218000	-0.00819600
C	3.88637600	-0.62574400	-1.41940100
C	3.60660000	0.94177100	-1.46143400
C	2.23918900	1.02401900	-2.01636800
C	1.38319700	2.09718700	-1.94007200
C	0.09792800	1.97952400	-2.40591000
C	-0.32565400	0.79369500	-2.95474900
C	-1.72363000	0.42261500	-3.27030900
C	-1.63829700	-1.14425200	-3.17239200

C	-0.14455200	-1.50307200	-3.51332300
C	0.50924800	-2.78078100	-2.88097000
C	2.02063700	-2.54085800	-2.25679000
C	2.82775500	-1.23658700	-2.52903800
C	1.83444400	-0.14487900	-2.61311100
C	0.54148500	-0.26883700	-3.06203800
C	-3.29728600	1.27082300	0.05922300
C	-2.07007700	2.03455400	-0.15115200
C	-1.76998300	3.10471500	0.82754700
C	-0.38234500	3.76296400	0.54979100
C	0.49397300	2.88122100	1.35972000
C	1.78619700	2.50606300	1.07684200
C	2.36049500	1.45210900	1.74862100
C	1.67015900	0.81370500	2.75304900
C	2.06586400	-0.46023900	3.39583700
C	0.60150200	-1.07162500	3.85707500
C	0.10470400	-2.33658800	3.07301400
C	-1.39162300	-2.44704900	2.57140600
C	-1.95909400	-1.10670300	2.27806200
C	-3.22924600	-0.97523600	1.51594300
C	-3.48372300	0.59595300	1.44463700
C	-2.51038500	1.18705300	2.56078600
C	-1.68354300	2.50281100	2.25695000
C	-0.21704600	2.22419700	2.34314400
C	0.38357800	1.20488200	3.04694700
C	-0.38995300	0.16525300	3.76576400
C	-1.59679600	0.01194400	2.88687500
F	-4.70398200	0.17268000	-1.51267800
F	-3.70047700	1.68668200	-3.13341400
F	-3.26508900	3.57557100	-1.69313600
F	-1.06101900	3.91311300	-3.05314800
F	0.06915300	5.19263400	-1.26684300
F	2.23445900	4.26745000	-2.02531100
F	3.26164800	4.15204700	0.32752000
F	4.95006400	2.44613800	-0.27124600
F	4.62198500	1.70431500	2.01434300
F	5.22314900	-0.60207200	1.76195900
F	3.75086200	-2.09970100	3.08458100
F	-1.37820600	-4.62294700	1.61728200
F	-3.23699800	-4.12227600	0.15733000
F	-4.53506900	-2.08639300	-0.06397700
F	-2.56545000	-3.81326000	-2.18480200
F	-0.26862700	-4.79214400	-1.82426200
F	4.77810000	-2.25141100	0.02918700

F	5.13137400	-0.82763300	-1.88674400
F	4.45674200	1.45556300	-2.40046300
F	-2.01467000	0.73256800	-4.56255600
F	-2.47383600	-1.73415500	-4.06284400
F	-0.04691600	-1.60986500	-4.86812500
F	0.61003500	-3.70636200	-3.84916500
F	2.76423700	-3.61620800	-2.62134800
F	3.51419700	-1.36756300	-3.69265800
F	-2.72625900	4.09238500	0.84038700
F	-0.38756300	5.01278600	1.09712300
F	2.77046000	-0.23332300	4.53437000
F	0.70504400	-1.41360800	5.15362900
F	0.35811300	-3.43350100	3.84022100
F	-2.17288100	-3.05769300	3.49630200
F	-4.20738400	-1.52150600	2.29916200
F	-4.76806500	0.79645600	1.82919000
F	-3.27432800	1.42663000	3.65904800
F	-2.04225300	3.45268000	3.16229500
F	-0.77245600	0.54323300	5.01736100
H	-4.06633500	3.01157800	-0.85339100
O	-4.44164200	2.28354400	-0.08842700
H	-5.27671800	1.84327100	-0.35244800
PC			
C	-2.67123100	-1.01467900	-1.11112900
C	-3.36410500	0.28034500	-1.35528100
C	-2.59573800	1.17727800	-2.36762100
C	-1.92078700	2.17563200	-1.43749600
C	-0.80879600	3.05320100	-1.91423300
C	-0.01233700	3.88352400	-0.82444700
C	1.56062200	3.43337300	-1.04420900
C	2.46528100	3.08565200	0.16342100
C	3.66575900	1.97030200	0.03951300
C	3.56577800	1.17235300	1.41346200
C	3.90078400	-0.35257100	1.49711200
C	2.89913800	-1.20994100	2.48194300
C	2.06713300	-1.92549900	1.49331200
C	0.83110500	-2.47486200	1.72673000
C	0.11105800	-3.00535200	0.68338600
C	-1.25015900	-3.42507800	1.07499900
C	-2.25644500	-3.20339900	-0.11629200
C	-3.16677600	-1.91230900	-0.02691300
C	-1.84150100	-1.62945500	-1.94571800
C	-1.58220200	-3.05992100	-1.59201100
C	-0.08990100	-3.40999500	-1.79549100

C	0.63388900	-3.00650600	-0.58016300
C	1.86989900	-2.46181400	-0.81757500
C	2.56732600	-1.88618800	0.21550700
C	3.84805100	-1.15831100	0.12277600
C	3.97327000	-0.44674200	-1.26250300
C	3.63374900	1.10842300	-1.27140100
C	2.30228100	1.15979500	-1.91127200
C	1.41150200	2.20556500	-1.85764700
C	0.16581100	2.05792400	-2.41332500
C	-0.19867400	0.87452300	-3.02047200
C	-1.58844300	0.44656300	-3.34813300
C	-1.43671400	-1.11473200	-3.28142700
C	0.07986700	-1.41270300	-3.58387900
C	0.75577200	-2.68272400	-2.95456100
C	2.22459700	-2.40248900	-2.24960300
C	2.99512800	-1.06388600	-2.44644600
C	1.96997600	-0.00315000	-2.56400000
C	0.70883300	-0.15859300	-3.09669300
C	-3.52144900	1.13676100	-0.05993600
C	-2.36248400	2.08806500	-0.18851700
C	-2.02152800	3.06162000	0.87959400
C	-0.59569800	3.71789600	0.63018100
C	0.26705600	2.80004600	1.42186700
C	1.59225700	2.48835400	1.19775200
C	2.18395400	1.44554300	1.86936000
C	1.47953300	0.74923200	2.82407500
C	1.91221400	-0.51474700	3.46354300
C	0.45566000	-1.20499900	3.84141400
C	0.05797800	-2.45988300	2.98782900
C	-1.40872100	-2.62590800	2.41978600
C	-2.02761200	-1.30247800	2.14806700
C	-3.26441700	-1.20672100	1.32803100
C	-3.60255500	0.34463300	1.30731800
C	-2.70459800	0.95517700	2.47710800
C	-1.91956600	2.32306300	2.25845600
C	-0.45133500	2.07988700	2.35074200
C	0.16560600	1.07216300	3.06091300
C	-0.58647100	-0.00939700	3.73888100
C	-1.75102800	-0.18966300	2.81074500
F	-4.59986600	-0.01338900	-1.85343900
F	-3.50220000	1.84012600	-3.12993700
F	-2.75160600	5.16151400	-1.25337200
F	-1.24023900	3.87646700	-2.92857100
F	-0.08147300	5.18549600	-1.15745700

F	2.15824600	4.41282000	-1.77125300
F	3.03605800	4.22739100	0.62791900
F	4.83776700	2.62922400	0.04441000
F	4.40473700	1.80136900	2.28953200
F	5.15073500	-0.46279300	1.97851100
F	3.67754800	-2.07697700	3.17831900
F	-1.24450100	-4.75420300	1.36933700
F	-3.06878400	-4.27501000	-0.14496100
F	-4.43827300	-2.27432200	-0.37083500
F	-2.30645500	-3.83605400	-2.44157100
F	0.01336500	-4.75308500	-1.98353800
F	4.84930500	-2.08563200	0.17949500
F	5.24647600	-0.58453000	-1.66969100
F	4.51509000	1.68888200	-2.13872900
F	-1.90690300	0.77583000	-4.62633300
F	-2.21874500	-1.70838400	-4.21586900
F	0.21861000	-1.48912500	-4.93611300
F	0.94087400	-3.57349800	-3.94087700
F	3.02855400	-3.43847000	-2.59725000
F	3.74552300	-1.14040100	-3.57386700
F	-2.98571300	3.99709800	0.97474100
F	-0.61070300	4.94647300	1.21119600
F	2.54961900	-0.27353000	4.63641200
F	0.51204600	-1.58620200	5.12827800
F	0.34758100	-3.57184000	3.71785900
F	-2.19147500	-3.30816200	3.28941500
F	-4.23609400	-1.85885100	2.03541000
F	-4.90300300	0.43253600	1.70074600
F	-3.51581800	1.13088300	3.55105900
F	-2.30780600	3.19030200	3.22855700
F	-1.02200900	0.33197500	4.98187800
O	-4.63170800	1.96602300	-0.17385100
H	-5.43085200	1.45253600	0.02705100
H	-2.33726900	5.27073300	-2.07751600
IP			
C	2.80105800	1.01047800	-0.79731100
C	3.25618100	-0.06458400	-1.71811400
C	2.31994300	-0.21812400	-2.94983300
C	1.49902300	-1.43537100	-2.55692200
C	0.26300700	-1.81029700	-3.30550400
C	-0.63595600	-2.95606400	-2.67950800
C	-2.11391700	-2.25805500	-2.49166300
C	-2.91679900	-2.44425800	-1.17679200
C	-3.91497800	-1.27174600	-0.60873900

C	-3.65393500	-1.29606100	0.96342000
C	-3.71940800	0.00833100	1.82305000
C	-2.56344200	0.11125400	2.98806300
C	-1.64790500	1.10999800	2.40027800
C	-0.33227600	1.29760200	2.74179300
C	0.43998700	2.18257400	2.02895800
C	1.86216100	2.15755700	2.42777000
C	2.78553400	2.43307500	1.18314000
C	3.46917600	1.16555800	0.52821800
C	2.06487100	2.06435300	-1.12825300
C	2.06142300	3.14279900	-0.09151800
C	0.64503000	3.74654700	0.06155700
C	-0.10578700	2.88952200	0.99274400
C	-1.41884300	2.70048100	0.64529400
C	-2.17904400	1.78600800	1.33049800
C	-3.56557100	1.38068400	1.02559500
C	-3.84046200	1.48506900	-0.50972300
C	-3.77294700	0.11862700	-1.32339700
C	-2.49187900	0.21997600	-2.05715800
C	-1.78945800	-0.81744600	-2.62558700
C	-0.55095000	-0.57756600	-3.17062900
C	-0.00652500	0.69055600	-3.13962900
C	1.43185900	1.03361000	-3.34075300
C	1.54454300	2.35005900	-2.49283900
C	0.09561800	2.95941000	-2.45082000
C	-0.34125700	3.81552100	-1.20920400
C	-1.81453200	3.41570700	-0.58301400
C	-2.80525500	2.47778700	-1.33335900
C	-1.98327400	1.49728900	-2.07667200
C	-0.72803700	1.73079000	-2.59537800
C	3.29652900	-1.46907900	-1.03870500
C	1.98335500	-2.05082800	-1.48673500
C	1.50486800	-3.37470400	-1.02245000
C	-0.01262300	-3.61862900	-1.39786100
C	-0.68043900	-3.12929900	-0.17056600
C	-1.93828400	-2.57601900	-0.07452000
C	-2.33021500	-1.95009200	1.08330400
C	-1.49253200	-1.92997200	2.17571300
C	-1.68565600	-1.10801400	3.39344500
C	-0.12384700	-0.90187400	3.90090900
C	0.45815700	0.54451000	3.73894300
C	1.91776800	0.77546900	3.17794700
C	2.30570200	-0.30078700	2.22914100
C	3.48635400	-0.13550000	1.33901700

C	3.55240300	-1.49603900	0.52095100
C	2.58969800	-2.48497700	1.32468700
C	1.58213000	-3.44138900	0.54076700
C	0.17680900	-3.08560200	0.90596900
C	-0.24374400	-2.49626400	2.07897800
C	0.69785700	-2.00989700	3.11292800
C	1.85363700	-1.54558300	2.27556800
F	4.51261900	0.26544000	-2.13679600
F	3.08174900	-0.54078600	-4.02578100
F	0.57794900	-2.10917300	-4.59669900
F	-0.76376500	-3.92080000	-3.60838700
F	-2.88091600	-2.67328400	-3.53276700
F	-3.66174500	-3.57643600	-1.28078100
F	-5.18153400	-1.68234500	-0.80576800
F	-4.57422300	-2.15657400	1.49231400
F	-4.91902100	0.02844000	2.43039200
F	-3.17025300	0.60506600	4.09836700
F	2.09311700	3.14096300	3.34107700
F	3.76606800	3.25456700	1.60259200
F	4.77166600	1.48978800	0.27113200
F	2.88869200	4.13452400	-0.52005100
F	0.76970000	5.00580000	0.56034500
F	-4.39926500	2.27544600	1.63502100
F	-5.08217500	1.98042500	-0.65722000
F	-4.77039900	0.17966400	-2.25612200
F	1.68066500	1.35389100	-4.63698800
F	2.39219900	3.22580700	-3.08759800
F	-0.04672900	3.73061800	-3.56520500
F	-0.40265300	5.09860600	-1.60206700
F	-2.44215900	4.58269200	-0.28632800
F	-3.56539900	3.21795200	-2.18003500
F	2.27780800	-4.34664100	-1.56447500
F	-0.18893700	-4.96590400	-1.49965600
F	-2.32607500	-1.80839800	4.36310400
F	-0.08082200	-1.21537600	5.20794900
F	0.37909500	1.16197900	4.95015900
F	2.81786400	0.82057300	4.18937800
F	4.57821800	-0.06598900	2.16041400
F	4.82550800	-1.94987300	0.67355600
F	3.37976600	-3.28662900	2.08524100
F	1.85689400	-4.72448100	0.89151300
F	1.10411700	-2.98465200	3.97131800
O	4.24056100	-2.27083100	-1.67236600
H	5.12746700	-2.01995100	-1.36437100

C₁-S_N2'-C40-F_h

RC

C	-2.73712900	-1.13255400	-0.97542200
C	-3.36129800	0.20855100	-1.10044000
C	-2.84633700	1.11570700	-2.26808400
C	-2.35049000	2.46450800	-1.50630500
C	-0.99404200	3.09088400	-1.89733100
C	-0.15510700	3.91687700	-0.80939000
C	1.40502000	3.48122900	-1.11922600
C	2.41337500	3.17896800	0.02274300
C	3.62863200	2.07814400	-0.17589800
C	3.63555000	1.28351400	1.20335300
C	4.00438600	-0.23702000	1.26757900
C	3.08808200	-1.11254800	2.31136300
C	2.21844400	-1.86136000	1.38034300
C	1.01167200	-2.43652000	1.69170700
C	0.24341600	-2.99525700	0.69828400
C	-1.08088900	-3.44174600	1.17792200
C	-2.16659900	-3.26349600	0.04848000
C	-3.11756300	-1.99877100	0.18636400
C	-1.93678700	-1.72565400	-1.84615500
C	-1.59302400	-3.13107300	-1.47650500
C	-0.09903300	-3.42490700	-1.76313400
C	0.68838600	-2.99607000	-0.59528100
C	1.89652800	-2.42619900	-0.91112300
C	2.64158000	-1.82346500	0.07434400
C	3.89100000	-1.05340500	-0.09795400
C	3.90810000	-0.34288300	-1.48726800
C	3.52378000	1.20383800	-1.47250000
C	2.13942900	1.20302000	-1.98442900
C	1.21481600	2.20831800	-1.84512100
C	-0.07448200	2.00343200	-2.26100700
C	-0.43470900	0.81986900	-2.84724900
C	-1.80443300	0.39822700	-3.20824600
C	-1.61904600	-1.17368900	-3.18850100
C	-0.10304000	-1.41902800	-3.54584700
C	0.64466600	-2.67383400	-2.97240900
C	2.15397400	-2.35426800	-2.36439800
C	2.86737700	-0.98815700	-2.59905700
C	1.79513900	0.02961800	-2.61026700
C	0.50195000	-0.17041300	-3.02776000
C	-3.00881900	0.92034200	0.15878900
C	-2.37472400	2.06580900	-0.06240600
C	-1.99529200	3.04148300	0.98810000

C	-0.61025900	3.72543800	0.68065900
C	0.31755800	2.84160800	1.42806600
C	1.63389100	2.56959400	1.12467200
C	2.28386100	1.53506900	1.75318800
C	1.64956900	0.82098400	2.74405600
C	2.14954300	-0.43577200	3.35040500
C	0.74194800	-1.15981100	3.82057500
C	0.31942400	-2.42914400	2.99887900
C	-1.17695000	-2.63683700	2.52854300
C	-1.84947800	-1.33219300	2.30145700
C	-3.12777600	-1.23976200	1.53887200
C	-3.37958300	0.31650200	1.47458300
C	-2.52897000	0.92101700	2.63961000
C	-1.81514500	2.31644900	2.37448600
C	-0.33469400	2.11229400	2.39777300
C	0.34591900	1.11445000	3.06670800
C	-0.33128200	0.00824200	3.78541700
C	-1.54258800	-0.20603300	2.93312300
F	-4.71041300	0.02029800	-1.21688700
F	-3.91078800	1.45210900	-3.02489400
F	-3.29048000	3.43176000	-1.70260100
F	-1.19247300	3.90427700	-2.97212200
F	-0.28119400	5.22214000	-1.10343400
F	1.92273800	4.43323000	-1.93772000
F	2.99679300	4.33673100	0.42668400
F	4.78560800	2.75978500	-0.25435500
F	4.52260000	1.93047700	2.01730000
F	5.28435900	-0.31720100	1.67413600
F	3.93107700	-1.95362900	2.96567700
F	-1.02313300	-4.76693100	1.48926800
F	-2.94513700	-4.36084500	0.08360300
F	-4.39368500	-2.42438000	-0.03869400
F	-2.33075000	-3.96227800	-2.26186500
F	0.04213900	-4.76412900	-1.96110300
F	4.92646600	-1.94473000	-0.10043400
F	5.15419400	-0.44703000	-1.98094700
F	4.31275000	1.80251400	-2.41305000
F	-2.08145000	0.75965300	-4.49164200
F	-2.41620000	-1.77394200	-4.10533600
F	0.00524800	-1.45141600	-4.90318900
F	0.78911700	-3.55627900	-3.97404400
F	2.95941100	-3.36391400	-2.77884100
F	3.53223500	-1.02108400	-3.78089800
F	-2.95678300	3.99143700	1.05656300

F	-0.62762100	4.95435500	1.26987500
F	2.85677800	-0.17968100	4.48039700
F	0.89081100	-1.53493000	5.10311000
F	0.67990900	-3.52956700	3.71551900
F	-1.87671600	-3.34398000	3.44957700
F	-4.10384500	-1.79726600	2.31122000
F	-4.69654200	0.54994500	1.69536800
F	-3.33896300	1.06339600	3.71910200
F	-2.19946400	3.18219100	3.34704100
F	-0.70477500	0.33745700	5.05256400
H	-5.52376000	2.92000700	-1.04286500
O	-5.42703500	2.53118500	-0.16432400
H	-6.11104200	1.85094400	-0.12746900
TS	imaginary vibrational frequency		-810.03 cm ⁻¹
C	-2.75701200	-0.90967700	-1.02122400
C	-3.40074000	0.42264200	-1.24789900
C	-2.70476300	1.27059800	-2.38428200
C	-2.09534400	2.51409900	-1.58271700
C	-0.74591900	3.11305600	-1.98745500
C	0.09564900	3.89853000	-0.87728600
C	1.63754000	3.38024900	-1.12791700
C	2.58732500	3.04176700	0.05013800
C	3.73811700	1.86902000	-0.09780800
C	3.65869900	1.09976700	1.29209600
C	3.93471700	-0.43857800	1.38633200
C	2.94186200	-1.24525400	2.41300900
C	2.05845900	-1.96061900	1.46896600
C	0.81559100	-2.47046800	1.75295900
C	0.04287700	-2.98941000	0.74140200
C	-1.32419900	-3.33861800	1.17863600
C	-2.36131800	-3.09221700	0.01402600
C	-3.22697700	-1.76828600	0.10924000
C	-1.97818300	-1.57157900	-1.86816300
C	-1.73871000	-2.99831100	-1.48424000
C	-0.26392800	-3.40655000	-1.72541600
C	0.52017700	-3.02455700	-0.53977400
C	1.76608500	-2.52723700	-0.82556800
C	2.51813500	-1.96052800	0.17550600
C	3.81517600	-1.26807200	0.02918300
C	3.91854900	-0.58337200	-1.37004700
C	3.63067000	0.98310700	-1.38927300
C	2.27336200	1.06100700	-1.96214000
C	1.40932600	2.12300400	-1.87004800
C	0.13363500	1.99698800	-2.34987500

C	-0.28627600	0.82899000	-2.92749500
C	-1.67950000	0.47400500	-3.28798900
C	-1.58936400	-1.09313700	-3.21982800
C	-0.08581100	-1.44661500	-3.54120500
C	0.56572700	-2.73032300	-2.92102700
C	2.07075600	-2.49415100	-2.27106600
C	2.87842400	-1.18342000	-2.50839900
C	1.87892100	-0.09784100	-2.58640600
C	0.58993400	-0.22338300	-3.05042800
C	-3.30297200	1.25466200	0.03829800
C	-2.07035400	2.01520400	-0.17811100
C	-1.75253800	2.94530900	0.80952200
C	-0.44915800	3.75062100	0.58948100
C	0.44721300	2.89075700	1.42940600
C	1.74554900	2.51819900	1.15193600
C	2.31391300	1.44781300	1.80749500
C	1.61911600	0.78627000	2.79200900
C	2.01772100	-0.49858600	3.41450400
C	0.55627300	-1.13189800	3.84657500
C	0.08099800	-2.39147800	3.03470000
C	-1.40649300	-2.50958600	2.51049900
C	-1.97394100	-1.16898000	2.23124100
C	-3.23158600	-1.03185400	1.45122200
C	-3.48123800	0.52704800	1.40405400
C	-2.54502200	1.10858700	2.54390200
C	-1.74358100	2.43411800	2.25798900
C	-0.26816200	2.20028700	2.39238600
C	0.32781300	1.16628300	3.08113500
C	-0.44312600	0.09822400	3.76457100
C	-1.62755600	-0.05808400	2.86224500
F	-4.70432200	0.19439000	-1.57760800
F	-3.68476800	1.71233100	-3.19955500
F	-3.00279400	3.54704800	-1.75722600
F	-0.91305900	3.94376400	-3.05506600
F	0.05914600	5.20868300	-1.18165600
F	2.23623900	4.30391800	-1.92616400
F	3.23198500	4.17203400	0.44162800
F	4.93489000	2.48324900	-0.14711700
F	4.56513400	1.70562800	2.11819900
F	5.19552700	-0.58663600	1.83268700
F	3.71666000	-2.12063700	3.10568300
F	-1.37322700	-4.66095900	1.50244700
F	-3.21486000	-4.13383200	0.03150800
F	-4.52381700	-2.10186500	-0.16022900

F	-2.51175700	-3.77534300	-2.29101000
F	-0.22493300	-4.75577200	-1.90254500
F	4.79427300	-2.22069800	0.07565500
F	5.17191400	-0.77267000	-1.81935700
F	4.49546300	1.51922600	-2.30161900
F	-1.92193400	0.80939900	-4.58597100
F	-2.40798200	-1.67293600	-4.13264900
F	0.03728000	-1.52872700	-4.89564600
F	0.68363400	-3.64260000	-3.89973500
F	2.82162400	-3.56275400	-2.64025900
F	3.58541800	-1.29233200	-3.66170500
F	-3.07611900	4.02995200	0.88648400
F	-0.55655900	4.98808600	1.14173100
F	2.70533900	-0.28351400	4.56579300
F	0.64520300	-1.49449700	5.13864000
F	0.33778000	-3.49680100	3.78790200
F	-2.19692700	-3.13973000	3.41391500
F	-4.21391300	-1.60135800	2.21332000
F	-4.78518900	0.70563500	1.78646900
F	-3.32421400	1.32897200	3.63632300
F	-2.15910800	3.38860400	3.12866400
F	-0.85574400	0.44495900	5.01549100
O	-4.41088000	2.29380700	-0.00334700
H	-3.93362800	3.23521500	0.42322100
H	-5.20311500	1.98911700	0.48729900
IP			
C	2.90449500	0.16775600	0.96119000
C	3.40020200	1.39129500	0.26767300
C	2.68075800	2.72855700	0.70522300
C	1.92238700	3.24125500	-0.63689800
C	0.45979000	3.75479700	-0.53804000
C	-0.55703200	3.59695400	-1.77055600
C	-1.98356000	3.22867300	-1.06632000
C	-2.95334300	2.17425300	-1.67031300
C	-3.91888800	1.26680000	-0.68369900
C	-3.81324100	-0.19527900	-1.30490200
C	-3.87409500	-1.46714300	-0.39214700
C	-2.82674100	-2.65355600	-0.81249200
C	-1.81175200	-2.54532300	0.25574000
C	-0.52982800	-3.03032000	0.20090900
C	0.35074700	-2.75244800	1.21973500
C	1.72890600	-3.19678900	0.92502300
C	2.77801000	-2.20006500	1.55203300
C	3.44814200	-1.16514500	0.55650600

C	2.27817000	0.12531300	2.12972000
C	2.22156500	-1.23982500	2.74017300
C	0.82844200	-1.51390000	3.36203300
C	-0.05647500	-2.01482200	2.29761000
C	-1.34355400	-1.54349800	2.36571500
C	-2.20912500	-1.78006000	1.32375100
C	-3.57931100	-1.24981000	1.16369600
C	-3.70199200	0.15036800	1.84041300
C	-3.61738900	1.39399300	0.85035500
C	-2.24765500	1.89258000	1.07217100
C	-1.53249900	2.70850400	0.23676700
C	-0.22437900	3.00137800	0.52229000
C	0.36454600	2.50146200	1.65012100
C	1.79727700	2.58728700	2.00604400
C	1.91085700	1.32023400	2.93545300
C	0.48268900	1.13580100	3.58037700
C	-0.02114000	-0.29788000	3.97350900
C	-1.57790200	-0.63247600	3.50526300
C	-2.53578400	0.47464000	2.97093900
C	-1.67722900	1.42289700	2.23029800
C	-0.36372700	1.71192500	2.51080800
C	3.29828200	1.29191500	-1.27938200
C	2.04191500	2.06285500	-1.55287100
C	1.24303400	1.87088300	-2.58505900
C	-0.07023700	2.58345500	-2.84798400
C	-0.91783600	1.35230500	-2.96170300
C	-2.13057600	1.13842700	-2.34449700
C	-2.56942300	-0.14819100	-2.11234600
C	-1.83191300	-1.22282800	-2.55104400
C	-2.06664800	-2.63727200	-2.16790900
C	-0.55346800	-3.27962600	-2.28769400
C	0.12250900	-3.71487100	-0.93607600
C	1.63554000	-3.37243600	-0.63422000
C	2.03175000	-2.10847300	-1.30126800
C	3.30597100	-1.42859200	-0.94270600
C	3.37034800	-0.16798800	-1.91004400
C	2.25926300	-0.48681000	-3.00903000
C	1.31182500	0.66116100	-3.47904100
C	-0.14542300	0.26958800	-3.37394700
C	-0.61994500	-1.00993200	-3.17700200
C	0.27429300	-2.19437900	-3.09582200
C	1.49003000	-1.64640800	-2.41563700
F	4.72520300	1.49334100	0.60473400
F	3.64731000	3.62569900	0.98161700

F	2.66134000	4.26518300	-1.14189100
F	0.50132800	5.07592200	-0.20867800
F	-0.68850800	4.79705000	-2.36074500
F	-2.65820900	4.39792200	-0.90189100
F	-3.77292000	2.78891800	-2.56105900
F	-5.18452000	1.68696600	-0.86526900
F	-4.84635200	-0.30999600	-2.19276700
F	-5.12009300	-1.96467100	-0.49527900
F	-3.50068700	-3.82925800	-0.70896500
F	1.93983000	-4.42437600	1.47505300
F	3.76249100	-2.95561300	2.07429000
F	4.78658000	-1.14782200	0.82923200
F	3.13437100	-1.27524800	3.74932000
F	0.97608900	-2.45129000	4.33671900
F	-4.42546300	-2.08629800	1.83504500
F	-4.89491000	0.19913800	2.45725800
F	-4.47981100	2.33325000	1.34146300
F	2.01689500	3.68837600	2.77671400
F	2.84239100	1.49761400	3.90202600
F	0.42296500	1.91753700	4.69333300
F	0.03245600	-0.39495800	5.31174000
F	-2.16544800	-1.27779500	4.54380100
F	-3.16201100	1.07635100	4.01253100
F	0.00461500	3.22108000	-4.05378000
F	-2.83124300	-3.26121900	-3.10106100
F	-0.64619300	-4.37413600	-3.06459300
F	-0.02707400	-5.06259900	-0.80963000
F	2.45025500	-4.37233300	-1.04850200
F	4.30745500	-2.29551500	-1.28389500
F	4.57769000	-0.23543700	-2.52166400
F	2.88896900	-0.96256800	-4.11781600
F	1.65286700	1.04106500	-4.74260100
F	0.63326800	-2.68633500	-4.31377600
O	4.28939200	2.09043500	-1.84410100
H	5.15874000	1.76800900	-1.55168700

C₁-S_N2'-C41-F_r

RC

C	-2.73717700	-1.13338500	-0.97565000
C	-3.36120800	0.20770100	-1.10130700
C	-2.84588600	1.11413300	-2.26937300
C	-2.35034100	2.46335200	-1.50814900
C	-0.99408700	3.09000700	-1.89929600
C	-0.15522600	3.91647400	-0.81146600
C	1.40483000	3.48071500	-1.12075000

C	2.41310700	3.17929000	0.02155900
C	3.62844900	2.07842500	-0.17628600
C	3.63523900	1.28450700	1.20337600
C	4.00411100	-0.23601100	1.26841300
C	3.08773200	-1.11115600	2.31244500
C	2.21850800	-1.86076700	1.38170300
C	1.01185500	-2.43614500	1.69317500
C	0.24378600	-2.99545300	0.69985800
C	-1.08075600	-3.44137200	1.17939500
C	-2.16622100	-3.26364700	0.04954400
C	-3.11741400	-1.99901200	0.18658800
C	-1.93618800	-1.72663300	-1.84570900
C	-1.59232200	-3.13180300	-1.47531300
C	-0.09829600	-3.42583600	-1.76148700
C	0.68895400	-2.99666400	-0.59365100
C	1.89706100	-2.42672400	-0.90954100
C	2.64185500	-1.82341100	0.07574400
C	3.89112300	-1.05309800	-0.09672100
C	3.90837000	-0.34324000	-1.48636200
C	3.52379700	1.20340700	-1.47234900
C	2.13949600	1.20208300	-1.98437200
C	1.21479300	2.20741300	-1.84595200
C	-0.07431600	2.00242300	-2.26238900
C	-0.43417900	0.81850100	-2.84819800
C	-1.80376400	0.39633100	-3.20903600
C	-1.61820400	-1.17548200	-3.18829700
C	-0.10213600	-1.42089000	-3.54527800
C	0.64565700	-2.67527000	-2.97094100
C	2.15469300	-2.35528400	-2.36280300
C	2.86791700	-0.98918700	-2.59799100
C	1.79556500	0.02842400	-2.60986700
C	0.50258100	-0.17186500	-3.02782800
C	-3.00910100	0.92018800	0.15769700
C	-2.37486400	2.06558900	-0.06396200
C	-1.99571400	3.04183100	0.98611800
C	-0.61066200	3.72579300	0.67857100
C	0.31710100	2.84252100	1.42672200
C	1.63355700	2.57055800	1.12377100
C	2.28350100	1.53637100	1.75292200
C	1.64900500	0.82259300	2.74385200
C	2.14894000	-0.43384600	3.35083500
C	0.74147100	-1.15778700	3.82109500
C	0.31914900	-2.42772300	3.00012200
C	-1.17701800	-2.63545900	2.52934000

C	-1.84926400	-1.33097400	2.30114300
C	-3.12757600	-1.23929800	1.53860700
C	-3.37999100	0.31681600	1.47380300
C	-2.52940800	0.92207700	2.63855600
C	-1.81575200	2.31751600	2.37291000
C	-0.33527300	2.11365000	2.39670700
C	0.34531700	1.11619200	3.06627400
C	-0.33189400	0.01011300	3.78520800
C	-1.54284500	-0.20457900	2.93257600
F	-4.71048300	0.02021900	-1.21769800
F	-3.91007900	1.44996300	-3.02684500
F	-3.29110400	3.42994900	-1.70497700
F	-1.19271400	3.90294000	-2.97428200
F	-0.28130200	5.22162700	-1.10613600
F	1.92270900	4.43213000	-1.93986400
F	2.99632900	4.33737700	0.42478500
F	4.78540900	2.76009800	-0.25490200
F	4.52213500	1.93197500	2.01709700
F	5.28402300	-0.31596900	1.67524900
F	3.93067800	-1.95167500	2.96752600
F	-1.02342300	-4.76634000	1.49171700
F	-2.94466400	-4.36106000	0.08494700
F	-4.39350400	-2.42485200	-0.03816300
F	-2.32982100	-3.96329100	-2.26060400
F	0.04273400	-4.76514900	-1.95887600
F	4.92673000	-1.94426200	-0.09849800
F	5.15454200	-0.44736200	-1.97985600
F	4.31259800	1.80173000	-2.41329100
F	-2.08083300	0.75701200	-4.49262100
F	-2.41522500	-1.77634700	-4.10491000
F	0.00636200	-1.45407900	-4.90256800
F	0.79040400	-3.55826500	-3.97207500
F	2.96043700	-3.36497600	-2.77663900
F	3.53289100	-1.02256100	-3.77974200
F	-2.95727600	3.99165900	1.05399800
F	-0.62834200	4.95502400	1.26708700
F	2.85603200	-0.17697500	4.48077100
F	0.89021700	-1.53222000	5.10385800
F	0.67916700	-3.52767500	3.71772000
F	-1.87749500	-3.34163700	3.45062100
F	-4.10317400	-1.79708500	2.31145000
F	-4.69687700	0.54971200	1.69495700
F	-3.33940400	1.06481000	3.71798400
F	-2.20042200	3.18373400	3.34489800

F	-0.70582800	0.33966600	5.05214400
H	-5.51884800	2.91661200	-1.04207100
O	-5.42924400	2.53176600	-0.16108600
H	-6.11266700	1.85071700	-0.12742800
TS	imaginary vibrational frequency		-827.96 cm ⁻¹
C	-2.79704400	-1.17344100	-1.02674600
C	-3.10365900	0.24592800	-1.04970300
C	-2.81514700	1.09954800	-2.28316700
C	-2.42422400	2.53328000	-1.59485100
C	-0.99647500	3.07814400	-1.89200500
C	-0.18115500	3.90736500	-0.81527200
C	1.38708800	3.47598400	-1.11151700
C	2.38040900	3.16988700	0.03715400
C	3.60391700	2.07425200	-0.15117600
C	3.59438900	1.27789100	1.22611200
C	3.96983400	-0.24121200	1.29453600
C	3.04906300	-1.11917700	2.33192500
C	2.18601600	-1.86908400	1.39483300
C	0.97785800	-2.44622800	1.69696000
C	0.21128200	-2.99659800	0.69624700
C	-1.11219900	-3.45585400	1.16419100
C	-2.19940600	-3.28247700	0.02508300
C	-3.14680700	-2.01713500	0.15787300
C	-2.00165700	-1.77737700	-1.90500600
C	-1.62525300	-3.16747700	-1.50808800
C	-0.11348400	-3.43000400	-1.76730500
C	0.65963200	-2.98813500	-0.59470000
C	1.87446300	-2.42590900	-0.89958200
C	2.61602600	-1.82771300	0.09130300
C	3.86849000	-1.05955000	-0.06988500
C	3.90131600	-0.35026600	-1.45866000
C	3.51674100	1.19849600	-1.44929700
C	2.13618000	1.19498000	-1.97012700
C	1.20439200	2.19394800	-1.82309500
C	-0.08651200	1.97078800	-2.21663800
C	-0.42783300	0.79441900	-2.82173400
C	-1.78294300	0.38952000	-3.21757300
C	-1.62714800	-1.19043400	-3.22027700
C	-0.09694000	-1.43245000	-3.54570000
C	0.64296100	-2.68593100	-2.96990300
C	2.14926900	-2.36319900	-2.34936500
C	2.87093000	-0.99821800	-2.57892400
C	1.79939900	0.01868400	-2.59519500
C	0.50743100	-0.19023400	-3.01041000

C	-2.68719900	0.86326300	0.13011500
C	-2.78320000	2.29740000	-0.09429300
C	-2.11682200	3.13958200	1.00602100
C	-0.65570200	3.70626000	0.65630400
C	0.24945900	2.78735200	1.38233800
C	1.57903400	2.54054300	1.11008000
C	2.23155400	1.51735300	1.75155200
C	1.59254800	0.80354800	2.73879400
C	2.10125000	-0.44249400	3.36123900
C	0.70032500	-1.17454100	3.83044500
C	0.28430400	-2.44869100	3.00328600
C	-1.20866200	-2.66341500	2.52530900
C	-1.86732100	-1.35722700	2.29766700
C	-3.11985600	-1.23785800	1.49868300
C	-3.26962500	0.30436000	1.38965600
C	-2.55196900	0.89063000	2.61586600
C	-1.87499300	2.29797700	2.36498200
C	-0.40048300	2.07391000	2.35599900
C	0.28629500	1.09182600	3.05058900
C	-0.37391300	-0.00955600	3.79510800
C	-1.57531500	-0.23544300	2.94593200
F	-4.84413300	0.44219900	-1.00184500
F	-3.91423300	1.31955800	-3.03344500
F	-3.28382100	3.47868400	-2.08363400
F	-1.10049300	3.86650500	-3.00465600
F	-0.31763400	5.21237600	-1.11210800
F	1.90517200	4.42661000	-1.92975700
F	2.95344800	4.32330600	0.46806300
F	4.75863800	2.76077000	-0.21507400
F	4.46469700	1.92833000	2.05555600
F	5.24770200	-0.31467900	1.71001300
F	3.89024100	-1.95646000	2.99382300
F	-1.04379600	-4.78436300	1.46272700
F	-2.97939400	-4.37935800	0.07063300
F	-4.43163100	-2.42975700	-0.03842900
F	-2.31991000	-4.05274800	-2.27458400
F	0.05437200	-4.76984200	-1.94913600
F	4.90373400	-1.95163000	-0.06043000
F	5.15249400	-0.45384900	-1.93959200
F	4.31653000	1.79703100	-2.38045900
F	-2.02821600	0.77981000	-4.49963800
F	-2.39207600	-1.74758700	-4.19061900
F	0.03831300	-1.45408600	-4.90144100
F	0.79552200	-3.56955100	-3.96956900

F	2.95710700	-3.37675300	-2.75004800
F	3.54593300	-1.03180000	-3.75504900
F	-2.90944300	4.20357300	1.27034000
F	-0.57948300	4.92632000	1.26565700
F	2.80080000	-0.16733300	4.49218500
F	0.85010200	-1.55238100	5.11248700
F	0.65448100	-3.54668200	3.71930200
F	-1.91409200	-3.37566200	3.43894000
F	-4.13377100	-1.73103900	2.27129500
F	-4.60603700	0.60191700	1.51875200
F	-3.42269600	1.01420100	3.65111600
F	-2.21583700	3.12112400	3.39162300
F	-0.73845100	0.33668500	5.06074600
H	-4.52669700	3.38290700	-0.55898000
O	-4.29979900	2.58034600	-0.04375200
H	-4.75559700	1.65463200	-0.48064600
IP			
C	-2.58059300	-1.08619300	-1.18385100
C	-2.69426600	0.32093700	-1.30064200
C	-2.48634800	1.03952800	-2.58474800
C	-2.19527700	2.54436800	-2.06773900
C	-0.70170300	3.00297700	-2.22998900
C	0.04375800	3.85484000	-1.11851600
C	1.60848100	3.33547600	-1.20722400
C	2.44985400	3.05557300	0.06517300
C	3.63022400	1.90400000	0.08705800
C	3.43453200	1.20761600	1.50916400
C	3.71624900	-0.31722700	1.72051600
C	2.63884500	-1.07886700	2.70365800
C	1.84368800	-1.84745900	1.72361000
C	0.58425600	-2.35466600	1.92478700
C	-0.09058500	-2.94733400	0.88293700
C	-1.47842900	-3.31185600	1.23134600
C	-2.41653700	-3.17623100	-0.02508500
C	-3.24012200	-1.83621400	-0.08449700
C	-1.87948600	-1.84079700	-2.02122200
C	-1.67491800	-3.22557100	-1.50636000
C	-0.15104000	-3.55184500	-1.57538800
C	0.49825000	-3.05386700	-0.34863200
C	1.75941200	-2.54991800	-0.55062200
C	2.41479300	-1.91595800	0.47756000
C	3.71677800	-1.22016000	0.40642200
C	3.93942800	-0.61082900	-1.01523300
C	3.64083700	0.94972400	-1.15541000

C	2.33322900	0.97854200	-1.84332400
C	1.44051500	2.02431800	-1.86802800
C	0.19346800	1.83974300	-2.40638800
C	-0.12521500	0.64295600	-2.99286900
C	-1.46969800	0.25759400	-3.45382400
C	-1.36913700	-1.33795100	-3.32913100
C	0.16589600	-1.66038900	-3.47805100
C	0.76873100	-2.90349300	-2.73093200
C	2.20106000	-2.60088600	-1.95939200
C	3.01170100	-1.28996800	-2.20170700
C	2.01100300	-0.22453300	-2.42460900
C	0.77118400	-0.39887700	-2.98815100
C	-2.96316700	1.09552800	-0.25951800
C	-2.84498200	2.54908600	-0.59594900
C	-2.10136300	3.33659400	0.53772800
C	-0.58412800	3.77039500	0.30267100
C	0.16690300	2.83204000	1.15870700
C	1.50563900	2.52322700	1.07036600
C	2.03498300	1.53718400	1.86136400
C	1.25357300	0.92630600	2.81721500
C	1.62028800	-0.29159700	3.57771600
C	0.13348200	-0.92149900	3.92543400
C	-0.25214400	-2.22817500	3.13990300
C	-1.69348600	-2.40908500	2.51195600
C	-2.27273200	-1.09370800	2.13619000
C	-3.41812300	-0.99153600	1.19294300
C	-3.56530100	0.56793100	1.00248300
C	-2.87649700	1.20815200	2.23576700
C	-2.07005900	2.55129900	1.95347500
C	-0.62284800	2.22797500	2.09887900
C	-0.06612300	1.28483100	2.94289200
C	-0.86894200	0.28626100	3.68750400
C	-1.99418500	0.05953000	2.73283000
F	-3.67667800	1.06354800	-3.24620500
F	-2.93376200	3.39888600	-2.81108900
F	-0.63643800	3.73549000	-3.38268700
F	0.01334900	5.14542500	-1.49956500
F	2.26582700	4.21035100	-2.00999000
F	3.02286800	4.20725500	0.49953100
F	4.81664300	2.53646700	0.11034300
F	4.24448000	1.87748800	2.38207600
F	4.93347200	-0.42581700	2.28161700
F	3.35826700	-1.90842300	3.50234200
F	-1.51999400	-4.61320900	1.63306700

F	-3.28549600	-4.20276100	0.01655700
F	-4.49357800	-2.13278500	-0.54213300
F	-2.33243300	-4.13995400	-2.26182500
F	-0.00724100	-4.90245900	-1.65998700
F	4.69228900	-2.15939000	0.58774700
F	5.22971600	-0.80694600	-1.33872500
F	4.57574800	1.44390100	-2.01943700
F	-1.66228900	0.56216500	-4.76422900
F	-2.06051500	-1.93621500	-4.32856800
F	0.43419800	-1.80240000	-4.80574100
F	0.99075900	-3.85677100	-3.65115400
F	3.00012000	-3.67416300	-2.18733200
F	3.81479600	-1.44916000	-3.28393600
F	-2.79500100	4.49076600	0.71625600
F	-0.44132600	5.00987400	0.86439200
F	2.20140600	0.02227900	4.76307200
F	0.11532700	-1.21451100	5.23726700
F	-0.02579800	-3.28704300	3.96634800
F	-2.52650300	-3.03042200	3.38157200
F	-4.53384100	-1.44539100	1.83627600
F	-4.88380800	0.88824000	0.99988500
F	-3.81630500	1.46269500	3.17899400
F	-2.43276400	3.44789300	2.90864300
F	-1.34626800	0.75144500	4.87409800
O	-4.15446300	3.00101000	-0.67793200
H	-4.15899800	3.96774400	-0.77121300

C₁- S_N2'-C41-F_e

RC

C	-2.73717700	-1.13338500	-0.97565000
C	-3.36120800	0.20770100	-1.10130700
C	-2.84588600	1.11413300	-2.26937300
C	-2.35034100	2.46335200	-1.50814900
C	-0.99408700	3.09000700	-1.89929600
C	-0.15522600	3.91647400	-0.81146600
C	1.40483000	3.48071500	-1.12075000
C	2.41310700	3.17929000	0.02155900
C	3.62844900	2.07842500	-0.17628600
C	3.63523900	1.28450700	1.20337600
C	4.00411100	-0.23601100	1.26841300
C	3.08773200	-1.11115600	2.31244500
C	2.21850800	-1.86076700	1.38170300
C	1.01185500	-2.43614500	1.69317500
C	0.24378600	-2.99545300	0.69985800
C	-1.08075600	-3.44137200	1.17939500

C	-2.16622100	-3.26364700	0.04954400
C	-3.11741400	-1.99901200	0.18658800
C	-1.93618800	-1.72663300	-1.84570900
C	-1.59232200	-3.13180300	-1.47531300
C	-0.09829600	-3.42583600	-1.76148700
C	0.68895400	-2.99666400	-0.59365100
C	1.89706100	-2.42672400	-0.90954100
C	2.64185500	-1.82341100	0.07574400
C	3.89112300	-1.05309800	-0.09672100
C	3.90837000	-0.34324000	-1.48636200
C	3.52379700	1.20340700	-1.47234900
C	2.13949600	1.20208300	-1.98437200
C	1.21479300	2.20741300	-1.84595200
C	-0.07431600	2.00242300	-2.26238900
C	-0.43417900	0.81850100	-2.84819800
C	-1.80376400	0.39633100	-3.20903600
C	-1.61820400	-1.17548200	-3.18829700
C	-0.10213600	-1.42089000	-3.54527800
C	0.64565700	-2.67527000	-2.97094100
C	2.15469300	-2.35528400	-2.36280300
C	2.86791700	-0.98918700	-2.59799100
C	1.79556500	0.02842400	-2.60986700
C	0.50258100	-0.17186500	-3.02782800
C	-3.00910100	0.92018800	0.15769700
C	-2.37486400	2.06558900	-0.06396200
C	-1.99571400	3.04183100	0.98611800
C	-0.61066200	3.72579300	0.67857100
C	0.31710100	2.84252100	1.42672200
C	1.63355700	2.57055800	1.12377100
C	2.28350100	1.53637100	1.75292200
C	1.64900500	0.82259300	2.74385200
C	2.14894000	-0.43384600	3.35083500
C	0.74147100	-1.15778700	3.82109500
C	0.31914900	-2.42772300	3.00012200
C	-1.17701800	-2.63545900	2.52934000
C	-1.84926400	-1.33097400	2.30114300
C	-3.12757600	-1.23929800	1.53860700
C	-3.37999100	0.31681600	1.47380300
C	-2.52940800	0.92207700	2.63855600
C	-1.81575200	2.31751600	2.37291000
C	-0.33527300	2.11365000	2.39670700
C	0.34531700	1.11619200	3.06627400
C	-0.33189400	0.01011300	3.78520800
C	-1.54284500	-0.20457900	2.93257600

F	-4.71048300	0.02021900	-1.21769800
F	-3.91007900	1.44996300	-3.02684500
F	-3.29110400	3.42994900	-1.70497700
F	-1.19271400	3.90294000	-2.97428200
F	-0.28130200	5.22162700	-1.10613600
F	1.92270900	4.43213000	-1.93986400
F	2.99632900	4.33737700	0.42478500
F	4.78540900	2.76009800	-0.25490200
F	4.52213500	1.93197500	2.01709700
F	5.28402300	-0.31596900	1.67524900
F	3.93067800	-1.95167500	2.96752600
F	-1.02342300	-4.76634000	1.49171700
F	-2.94466400	-4.36106000	0.08494700
F	-4.39350400	-2.42485200	-0.03816300
F	-2.32982100	-3.96329100	-2.26060400
F	0.04273400	-4.76514900	-1.95887600
F	4.92673000	-1.94426200	-0.09849800
F	5.15454200	-0.44736200	-1.97985600
F	4.31259800	1.80173000	-2.41329100
F	-2.08083300	0.75701200	-4.49262100
F	-2.41522500	-1.77634700	-4.10491000
F	0.00636200	-1.45407900	-4.90256800
F	0.79040400	-3.55826500	-3.97207500
F	2.96043700	-3.36497600	-2.77663900
F	3.53289100	-1.02256100	-3.77974200
F	-2.95727600	3.99165900	1.05399800
F	-0.62834200	4.95502400	1.26708700
F	2.85603200	-0.17697500	4.48077100
F	0.89021700	-1.53222000	5.10385800
F	0.67916700	-3.52767500	3.71772000
F	-1.87749500	-3.34163700	3.45062100
F	-4.10317400	-1.79708500	2.31145000
F	-4.69687700	0.54971200	1.69495700
F	-3.33940400	1.06481000	3.71798400
F	-2.20042200	3.18373400	3.34489800
F	-0.70582800	0.33966600	5.05214400
H	-5.51884800	2.91661200	-1.04207100
O	-5.42924400	2.53176600	-0.16108600
H	-6.11266700	1.85071700	-0.12742800
TS	imaginary vibrational frequency		-819.54 cm ⁻¹
C	-2.73953400	-1.26396500	-0.95193100
C	-3.24027000	0.10750800	-1.10580900
C	-2.84792000	0.90739600	-2.36533400
C	-2.46655900	2.39915000	-1.75965000

C	-1.03196700	2.92564800	-2.09638700
C	-0.20120900	3.83654300	-1.09034800
C	1.36469800	3.38875000	-1.35552800
C	2.36749400	3.17470800	-0.18825200
C	3.59292600	2.07344900	-0.29817500
C	3.59405200	1.38011500	1.13725800
C	3.97170100	-0.12914400	1.31673500
C	3.04962000	-0.93470900	2.41346000
C	2.18821600	-1.74849100	1.53051100
C	0.98099100	-2.30684400	1.87191200
C	0.22520700	-2.93466000	0.91151900
C	-1.09610000	-3.36514400	1.40772000
C	-2.17040800	-3.28599800	0.25732000
C	-3.12011500	-2.01636000	0.28222000
C	-1.95369900	-1.93165900	-1.77896000
C	-1.58676600	-3.28921400	-1.27927800
C	-0.07824000	-3.56298000	-1.51579600
C	0.68406500	-3.03063200	-0.37382800
C	1.89228900	-2.47851800	-0.71710800
C	2.62411600	-1.80223600	0.22955300
C	3.87248400	-1.04061200	0.01215500
C	3.89924100	-0.43128200	-1.42571900
C	3.50282200	1.10916900	-1.52846400
C	2.12046500	1.06008800	-2.04394400
C	1.18003600	2.05854200	-1.96830100
C	-0.11239800	1.80218600	-2.34436600
C	-0.44299800	0.58321100	-2.86541800
C	-1.79492500	0.14185600	-3.23739300
C	-1.61105200	-1.43673200	-3.13793500
C	-0.08073600	-1.68602800	-3.43973100
C	0.66862600	-2.89144100	-2.76895200
C	2.16765100	-2.51505400	-2.16882500
C	2.87379600	-1.16423300	-2.49607400
C	1.79379100	-0.15913500	-2.58496800
C	0.50397600	-0.40352400	-2.98568700
C	-2.69871200	0.85331600	0.04762000
C	-2.79398800	2.27901000	-0.24240300
C	-2.10298100	3.20559400	0.78742000
C	-0.65409400	3.74657800	0.39541100
C	0.25105600	2.88719800	1.18811200
C	1.57935700	2.62663100	0.93676000
C	2.23430700	1.65533000	1.65274500
C	1.59441700	1.00838400	2.68598300
C	2.09895600	-0.19232700	3.39374400

C	0.69269000	-0.89139700	3.90624300
C	0.27843100	-2.21821000	3.17146000
C	-1.21619400	-2.47508800	2.70412800
C	-1.89251400	-1.19354400	2.39339200
C	-3.13728100	-1.11945700	1.55500000
C	-3.14732400	0.40220400	1.29357400
C	-2.55680000	1.08143500	2.51869900
C	-1.86998000	2.46086400	2.19680300
C	-0.39892100	2.23920600	2.20653900
C	0.28338200	1.30842000	2.96692900
C	-0.38436600	0.26412900	3.78307100
C	-1.58984500	-0.02694600	2.95445200
F	-4.63872500	0.04149400	-1.09526400
F	-3.94117300	1.09351900	-3.13858900
F	-3.34223900	3.29044500	-2.30772600
F	-1.15008700	3.63106800	-3.26112500
F	-0.34130800	5.11472900	-1.48554500
F	1.88283900	4.27438800	-2.24391300
F	2.93676800	4.36092000	0.14765500
F	4.74641900	2.75536800	-0.41529000
F	4.46870900	2.09274100	1.90870300
F	5.24885900	-0.17299500	1.73791800
F	3.89019800	-1.72459700	3.13101000
F	-1.01877000	-4.66556200	1.81100100
F	-2.94894200	-4.37800500	0.38524600
F	-4.39651800	-2.45830300	0.09489200
F	-2.28113300	-4.23104300	-1.97465500
F	0.10543100	-4.90944300	-1.60734400
F	4.91206400	-1.92457500	0.08135500
F	5.15094000	-0.56145900	-1.89912400
F	4.29268900	1.64598900	-2.50573000
F	-2.03569200	0.44142000	-4.54531500
F	-2.37499800	-2.06300500	-4.06593200
F	0.07213000	-1.80323300	-4.78856300
F	0.83147900	-3.84020900	-3.70579400
F	2.98572700	-3.54688800	-2.49660200
F	3.54895200	-1.27620400	-3.66747200
F	-2.87453300	4.29149600	0.99809000
F	-0.56649100	5.00833400	0.91229200
F	2.79363500	0.15485400	4.50709400
F	0.83800900	-1.17630400	5.21209100
F	0.64428100	-3.26314600	3.96532600
F	-1.92325100	-3.13176000	3.65704200
F	-4.18612400	-1.50232400	2.33271500

F	-4.78050100	0.91703800	1.41457400
F	-3.46687900	1.25897100	3.50631200
F	-2.21802800	3.33878400	3.17444800
F	-0.75445400	0.70161200	5.01888700
H	-4.70889100	1.83489600	0.59723000
O	-4.27863700	2.64217600	-0.09187600
H	-4.72331400	2.72429500	-0.95956600
IP			
C	-2.99513500	-0.92212000	-0.67518700
C	-3.49667600	0.47478200	-0.65934400
C	-3.11286700	1.38746000	-1.86346000
C	-2.53315300	2.78800400	-1.16981600
C	-1.09593800	3.22343300	-1.60806000
C	-0.09039800	3.95400100	-0.62064900
C	1.39555500	3.43487100	-1.12016900
C	2.50959700	3.02111100	-0.12048700
C	3.62693700	1.86516100	-0.50049300
C	3.74350600	1.01452800	0.84317200
C	4.01846400	-0.52690400	0.81369000
C	3.17445600	-1.39193300	1.92876900
C	2.14743000	-2.03490800	1.08300700
C	0.95065800	-2.54994500	1.51762900
C	0.03612900	-3.00868500	0.60092900
C	-1.24503000	-3.41068100	1.21227800
C	-2.43673800	-3.11922000	0.21941700
C	-3.26789000	-1.80475700	0.50483700
C	-2.35453500	-1.53714300	-1.65541300
C	-2.04396100	-2.97046100	-1.36141400
C	-0.60831100	-3.32873600	-1.82003700
C	0.32571000	-2.98074600	-0.73631200
C	1.52309200	-2.47543400	-1.17307400
C	2.41558400	-1.96450600	-0.26137000
C	3.68869500	-1.27532900	-0.55579500
C	3.59275300	-0.51022500	-1.91344800
C	3.30981600	1.05277200	-1.80104600
C	1.87448700	1.15032100	-2.12976800
C	1.03387600	2.19205200	-1.82948700
C	-0.31055100	2.06417100	-2.05804800
C	-0.80020300	0.94281900	-2.66268000
C	-2.21819400	0.64489700	-2.92003200
C	-2.14658000	-0.93890000	-2.99893400
C	-0.69176600	-1.25796400	-3.52456800
C	0.03490700	-2.57915800	-3.08448200
C	1.62138000	-2.37297100	-2.64436800

C	2.39128100	-1.04581700	-2.91760000
C	1.38932000	0.02868300	-2.75647000
C	0.04602400	-0.07942400	-3.01788400
C	-2.95275100	1.12138500	0.56455300
C	-2.79661900	2.59969700	0.38749400
C	-1.80934600	3.25352300	1.41822200
C	-0.37239000	3.71249800	0.88808800
C	0.53872400	2.68873300	1.44516700
C	1.81322700	2.38836100	1.02037900
C	2.47651800	1.30999400	1.54919900
C	1.91587200	0.59064900	2.58292900
C	2.41208500	-0.70805100	3.09901800
C	1.02694700	-1.36954600	3.71828900
C	0.42660800	-2.57534400	2.90222200
C	-1.13133500	-2.69121000	2.61840200
C	-1.74613200	-1.34550900	2.55983600
C	-3.03636400	-1.06114700	1.84135800
C	-2.87364600	0.43614400	1.69597100
C	-2.20884600	0.95810500	2.92497100
C	-1.46140300	2.30569000	2.68401900
C	-0.03131700	1.97333700	2.46317700
C	0.66754000	0.93080000	3.04348600
C	0.03527900	-0.13735900	3.86029900
C	-1.29685200	-0.26412900	3.19877700
F	-4.87316700	0.44436600	-0.55969000
F	-4.25509800	1.73648300	-2.49387800
F	-3.35547800	3.77562600	-1.58857400
F	-1.24429600	4.04873600	-2.68896600
F	-0.16833300	5.27553300	-0.85161100
F	1.87273100	4.37408700	-1.97503600
F	3.20448000	4.11710900	0.27527500
F	4.80748400	2.48043900	-0.69178700
F	4.75600300	1.57654400	1.56743600
F	5.32836300	-0.70267200	1.06331800
F	4.03039400	-2.31551800	2.43652300
F	-1.22921700	-4.75399600	1.44115600
F	-3.28237300	-4.16258600	0.31946400
F	-4.58864000	-2.13362900	0.44676500
F	-2.90643700	-3.74869800	-2.06935700
F	-0.55853700	-4.66687500	-2.06577800
F	4.64923400	-2.23396900	-0.71368800
F	4.76488200	-0.66904900	-2.55155400
F	4.00938400	1.64275900	-2.81465400
F	-2.56768200	1.10263000	-4.15463400

F	-3.07003600	-1.43324000	-3.85666800
F	-0.72560400	-1.23321000	-4.88518300
F	0.00487500	-3.42806000	-4.12459500
F	2.30835000	-3.41717700	-3.17142100
F	2.91154100	-1.06516900	-4.16969200
F	-2.40240500	4.36221400	1.89807600
F	-0.08077400	4.88487500	1.52801900
F	3.26384300	-0.53559900	4.14113300
F	1.30945600	-1.81278400	4.95576900
F	0.81870600	-3.72404700	3.51982100
F	-1.74776400	-3.43519100	3.56834100
F	-4.06943400	-1.35975900	2.68901800
F	-3.09562600	1.10421500	3.94689900
F	-1.59105900	3.05953700	3.80776800
F	-0.10854400	0.21080300	5.16812200
O	-4.04201700	3.16217700	0.70011100
H	-4.72200300	2.80169700	0.10577300

C₁-S_N2'-C1-F_j

RC

C	-3.07116600	-0.46340700	-0.41228900
C	-3.33662400	0.97660300	-0.64307500
C	-2.83251300	1.56886800	-1.99918800
C	-1.91226200	2.83258400	-1.52640900
C	-0.53567600	3.05284400	-2.18625800
C	0.64096400	3.76079000	-1.35289300
C	1.98395200	2.91010800	-1.78525600
C	3.06326700	2.49965400	-0.74446700
C	3.94368700	1.11390900	-0.92033900
C	3.98739800	0.51537000	0.55507200
C	3.99778700	-1.02776200	0.81183400
C	3.08299300	-1.51199700	2.08855300
C	1.92119600	-2.11854700	1.40538500
C	0.68090000	-2.33491600	1.95359600
C	-0.34603300	-2.79111400	1.16134800
C	-1.64545200	-2.82971200	1.86234700
C	-2.82866800	-2.52050200	0.86393900
C	-3.43111800	-1.05084100	0.91750600
C	-2.57032500	-1.34088100	-1.26833600
C	-2.49274200	-2.72805400	-0.72228800
C	-1.16570400	-3.41590000	-1.13931000
C	-0.12562600	-3.05823400	-0.16174000
C	1.11461300	-2.85276000	-0.71104500
C	2.12459600	-2.34108600	0.06694000
C	3.47481700	-1.94369800	-0.38245700

C	3.43619000	-1.43442800	-1.85821500
C	3.43234400	0.14871000	-2.04270400
C	2.02380200	0.44102700	-2.37770500
C	1.38754600	1.65416200	-2.28407300
C	0.03495800	1.73358700	-2.50328500
C	-0.68095400	0.61405100	-2.84204600
C	-2.15733200	0.49976100	-2.94619100
C	-2.32810500	-1.06201900	-2.70839100
C	-0.97659500	-1.70672000	-3.19475000
C	-0.46600100	-3.03092900	-2.53288400
C	1.14900500	-3.02895400	-2.17711300
C	2.11103800	-1.92582400	-2.71538700
C	1.32099700	-0.67657900	-2.75581400
C	-0.03235700	-0.59284600	-2.96945000
C	-2.58613300	1.69098200	0.42527700
C	-1.78370100	2.63396500	-0.04815500
C	-1.03117300	3.60348200	0.78459600
C	0.40412100	3.87495400	0.19767800
C	1.20624100	2.87914300	0.95075800
C	2.35229700	2.24266100	0.52857100
C	2.83812600	1.16304600	1.22560100
C	2.22677100	0.75764700	2.39056300
C	2.50891300	-0.50194700	3.12036800
C	1.06288900	-0.78271400	3.87062600
C	0.22673600	-1.99458500	3.31918700
C	-1.33315200	-1.87229200	3.07179900
C	-1.70394800	-0.47965800	2.72278300
C	-3.03253700	-0.15633500	2.12627900
C	-2.90170900	1.38574600	1.85053100
C	-1.77146600	1.89234100	2.79684300
C	-0.80632100	3.02435400	2.23346100
C	0.56922700	2.45956700	2.09780000
C	1.09578600	1.40841700	2.82183600
C	0.30155700	0.60465700	3.78326700
C	-1.04357300	0.59705900	3.13068200
F	-4.66237900	1.24868400	-0.45064800
F	-3.88442400	2.09260600	-2.65634600
F	-2.63916700	3.96877900	-1.71789100
F	-0.72336100	3.76959200	-3.32861100
F	0.77973600	5.00866200	-1.83138900
F	2.57663800	3.60057300	-2.79336700
F	3.95519800	3.51347400	-0.60304400
F	5.20015500	1.46800800	-1.24530000
F	5.11753300	1.01506200	1.13892100

F	5.27221900	-1.38055100	1.05992900
F	3.80210200	-2.45601700	2.74854900
F	-1.84939500	-4.07911200	2.36643300
F	-3.82315300	-3.37273200	1.17535000
F	-4.78978600	-1.15843400	0.93508300
F	-3.50863100	-3.45161200	-1.26626900
F	-1.36584500	-4.76260200	-1.13591000
F	4.25474500	-3.06486700	-0.37461000
F	4.53074100	-1.91226400	-2.47655200
F	4.18330200	0.40828300	-3.15419900
F	-2.55828300	0.76984000	-4.21910400
F	-3.32146500	-1.60120100	-3.45543300
F	-1.08911300	-1.93254500	-4.53476100
F	-0.69365600	-4.03390700	-3.39725300
F	1.62678400	-4.25246700	-2.51958900
F	2.55099900	-2.27190400	-3.95138200
F	-1.73122200	4.76352900	0.83219200
F	0.76658100	5.12983100	0.58581800
F	3.42661700	-0.30074400	4.09988200
F	1.32309600	-1.02253100	5.16794200
F	0.43098200	-3.05247600	4.15176400
F	-2.03426300	-2.25506200	4.16653700
F	-3.96690900	-0.34341200	3.10202700
F	-4.07187700	2.00278700	2.15484500
F	-2.34994200	2.35925400	3.93251500
F	-0.81906900	4.06650400	3.10394500
F	0.21514500	1.17208100	5.01753500
H	-5.87434800	0.46779000	-2.33621600
O	-5.31557700	-0.31532400	-2.41579300
H	-5.43119000	-0.61205200	-3.32700300
TS	imaginary vibrational frequency		-814.88 cm ⁻¹
C	-3.41447400	-0.26205600	-0.84244200
C	-3.31845400	1.25102300	-0.82598000
C	-2.59143200	1.94790500	-2.04792600
C	-1.66753300	3.08033400	-1.34066900
C	-0.22454000	3.33543500	-1.85045700
C	0.90013100	3.87235700	-0.83215600
C	2.25160500	3.02453100	-1.25811100
C	3.21745800	2.43009300	-0.19442800
C	4.05297000	1.03189100	-0.47392800
C	3.94374500	0.25351800	0.91081700
C	3.86641000	-1.30954500	0.96920700
C	2.83284500	-1.90476500	2.09699300
C	1.71537800	-2.38303300	1.25577200

C	0.42911400	-2.62324500	1.67488800
C	-0.54261600	-2.95099100	0.75747300
C	-1.90243100	-2.95079700	1.34419300
C	-2.96853000	-2.43155400	0.28309400
C	-3.63664900	-0.99416200	0.51900400
C	-2.28983800	-0.92192700	-1.48465700
C	-2.37451500	-2.28105100	-1.17167500
C	-1.22401000	-3.14922300	-1.67213800
C	-0.22787400	-3.06416800	-0.57235900
C	1.05818000	-2.82244100	-0.99251000
C	2.01828000	-2.44761900	-0.08054300
C	3.41313100	-2.04761800	-0.36777900
C	3.52086400	-1.35528000	-1.76219400
C	3.60400200	0.23760000	-1.74550200
C	2.25004900	0.64894400	-2.16388400
C	1.66337700	1.87588900	-1.97484600
C	0.34149700	2.05425700	-2.30244900
C	-0.37880700	1.02707500	-2.84209600
C	-1.84421800	0.97865300	-3.03523800
C	-2.06704800	-0.55960700	-2.91231400
C	-0.76672300	-1.22259400	-3.45822100
C	-0.36959300	-2.64121100	-2.93366500
C	1.20515200	-2.77717900	-2.46123400
C	2.25826500	-1.66678400	-2.77570000
C	1.53931500	-0.37604100	-2.74333700
C	0.22235600	-0.19157700	-3.07105900
C	-2.54159800	1.70331500	0.36991500
C	-1.66799700	2.66445500	0.09502600
C	-0.96272100	3.49797800	1.10583100
C	0.52469500	3.79384100	0.68970700
C	1.23360900	2.68632000	1.37816000
C	2.39055700	2.05620100	0.97527900
C	2.76915500	0.87329900	1.56306900
C	2.04506300	0.35546700	2.61267000
C	2.21391200	-0.99812300	3.19479100
C	0.70375900	-1.29911700	3.78509900
C	-0.12828100	-2.39614000	3.02708200
C	-1.64685300	-2.15273300	2.66542000
C	-1.92545300	-0.71612900	2.44551900
C	-3.19888000	-0.24843000	1.82249600
C	-2.97940300	1.28703200	1.72976400
C	-1.92249600	1.62280200	2.82463800
C	-0.87769700	2.76070500	2.49043700
C	0.48581800	2.15866000	2.40760700

C	0.90791100	1.00215100	3.03293000
C	0.00436300	0.12342000	3.81431600
C	-1.27330400	0.26609100	3.05331800
F	-4.59029000	1.75472200	-0.71402700
F	-3.54088600	2.58892400	-2.75792900
F	-2.33922600	4.26229500	-1.42664100
F	-0.29734000	4.21553800	-2.88640200
F	1.12665800	5.16511100	-1.12115700
F	2.95739000	3.82099900	-2.10252000
F	4.13720500	3.36929800	0.14708600
F	5.34621500	1.36065400	-0.64867100
F	5.03947000	0.61599400	1.64273800
F	5.10143200	-1.75093200	1.27147200
F	3.46480100	-2.94892900	2.69443800
F	-2.24975700	-4.22009000	1.69199900
F	-3.96941200	-3.33426900	0.31341100
F	-4.98560200	-1.18310300	0.65849400
F	-3.76171900	-2.83016900	-2.05074900
F	-1.61861600	-4.42907500	-1.88835300
F	4.15360000	-3.19431400	-0.44008000
F	4.64332100	-1.80995300	-2.34858500
F	4.46624800	0.58260600	-2.74796900
F	-2.15095900	1.37520800	-4.30344900
F	-3.10326800	-0.91709600	-3.74003900
F	-0.84701500	-1.29036700	-4.81849400
F	-0.56750100	-3.52268600	-3.92864700
F	1.66177000	-3.96105300	-2.94701500
F	2.79300600	-1.90122400	-4.00170800
F	-1.64345600	4.66491000	1.23016200
F	0.87188900	4.97673700	1.27052600
F	3.05368400	-0.96076800	4.26178200
F	0.84216700	-1.70521300	5.05983800
F	-0.06115900	-3.54519300	3.75554100
F	-2.46026800	-2.60762000	3.65119300
F	-4.17577300	-0.47557100	2.75198400
F	-4.14546100	1.93212300	1.99996400
F	-2.58722800	1.97730900	3.95409900
F	-0.93952400	3.70255900	3.46633700
F	-0.17393400	0.53422700	5.10003100
H	-4.41948300	-1.70398400	-1.96126000
O	-4.63331700	-0.63677400	-1.69129800
H	-5.46213800	-0.54275600	-1.17641500
IP			
C	3.51777200	-0.15541700	1.34747100

C	3.46819500	1.13862600	0.51825300
C	2.80418900	2.41024200	1.17678700
C	2.07990900	3.13021800	-0.09427900
C	0.66658200	3.74047800	0.06335300
C	-0.32463700	3.81756100	-1.20388600
C	-1.79761100	3.42418900	-0.57312200
C	-2.79672200	2.49296400	-1.32140700
C	-3.83453200	1.50406600	-0.49540300
C	-3.77672100	0.13828400	-1.31063500
C	-3.92340000	-1.25231700	-0.59690100
C	-2.93403700	-2.43001400	-1.16964700
C	-1.95290100	-2.57033000	-0.07070700
C	-0.69870700	-3.13224800	-0.17054800
C	0.16180500	-3.09067900	0.90405800
C	1.56476800	-3.44781700	0.53522800
C	2.58159400	-2.49775100	1.31619800
C	3.55021800	-1.51901100	0.50600900
C	2.33029700	-0.31691300	2.23803000
C	1.85773700	-1.55421500	2.27137500
C	0.69907800	-2.01524300	3.10703900
C	-0.24994900	-2.49781200	2.07782800
C	-1.49610400	-1.92710100	2.17918800
C	-2.33713800	-1.94256800	1.08906200
C	-3.65712800	-1.28010800	0.97399600
C	-3.71293600	0.02380800	1.83495500
C	-3.55420000	1.39607800	1.03824600
C	-2.16378000	1.79189600	1.33685600
C	-1.40054300	2.70333400	0.65112600
C	-0.08484800	2.88350200	0.99383100
C	0.46151900	2.17062100	2.02579600
C	1.88418200	2.14093300	2.42478300
C	1.93640400	0.76160700	3.18480400
C	0.47132400	0.53518300	3.73675400
C	-0.11595300	-0.90712800	3.89998500
C	-1.68073700	-1.10481000	3.39814000
C	-2.55234800	0.11937200	2.99553700
C	-1.63241700	1.11113100	2.40305000
C	-0.31432200	1.28958300	2.73868800
C	2.80185800	0.99518900	-0.80640900
C	2.07260500	2.05457500	-1.13480000
C	1.54734300	2.34498500	-2.49672700
C	0.10185500	2.96117900	-2.44866900
C	-0.72900900	1.73712100	-2.59329200
C	-1.98308500	1.50895800	-2.06969100

C	-2.49823400	0.23413000	-2.04965900
C	-1.80367700	-0.80637000	-2.62173300
C	-2.13450100	-2.24573600	-2.48674900
C	-0.66092800	-2.95167700	-2.68037000
C	-0.03339500	-3.62017400	-1.40121900
C	1.48152200	-3.37014500	-1.02485700
C	1.94896000	-2.04345300	-1.48432900
C	3.25801300	-1.46682900	-1.03719500
C	3.24822200	-0.07877200	-1.73251500
C	2.30403400	-0.22564800	-2.96015400
C	1.42451200	1.03107400	-3.34801300
C	-0.01544500	0.69427400	-3.14333000
C	-0.56708800	-0.57142400	-3.17358800
C	0.23932900	-1.80906600	-3.31153900
C	1.47509700	-1.43481400	-2.56333600
F	4.78072100	1.46319000	0.24292500
F	3.79586200	3.22057700	1.59383400
F	2.91275500	4.11725700	-0.52264300
F	0.79829600	4.99795600	0.56460400
F	-0.37998300	5.10152200	-1.59458000
F	-2.41797100	4.59379000	-0.27158100
F	-3.55586100	3.23814300	-2.16441100
F	-5.07407900	2.00590600	-0.63849900
F	-4.77677600	0.20540700	-2.24016800
F	-5.19298100	-1.65527600	-0.79028700
F	-3.68629900	-3.55721900	-1.27517600
F	1.83750100	-4.73485400	0.87336400
F	3.37119600	-3.30800200	2.06806000
F	4.81144800	-1.99714400	0.62241500
F	1.10089500	-2.99519300	3.96275500
F	-4.58087600	-2.13592300	1.50466200
F	-4.91064000	0.04998000	2.44592400
F	-4.37969700	2.29551900	1.65198300
F	2.11745000	3.13132100	3.33029500
F	2.81253800	0.81832700	4.21428100
F	0.38720900	1.15618700	4.94646800
F	-0.07043300	-1.22255100	5.20663200
F	-2.32248100	-1.80224000	4.36921100
F	-3.15196300	0.61866400	4.10740500
F	2.39705400	3.21776500	-3.09270300
F	-0.04000900	3.73481500	-3.56133700
F	-2.90627700	-2.65598100	-3.52624800
F	-0.79701300	-3.91480900	-3.60951600
F	-0.20468200	-4.96713700	-1.50916500

F	2.28046500	-4.31730100	-1.57819500
F	4.21949700	-2.22145600	-1.65159000
F	4.50216800	0.23076000	-2.15686800
F	3.06103200	-0.56154600	-4.03521200
F	1.67482100	1.35078300	-4.64356100
F	0.55338800	-2.11070300	-4.60152100
O	4.59704300	-0.09519300	2.22027600
H	5.39585200	0.12933400	1.71344700

C₁-S_N2'-C1-F_k

RC

C	-3.07116600	-0.46340700	-0.41228900
C	-3.33662400	0.97660300	-0.64307500
C	-2.83251300	1.56886800	-1.99918800
C	-1.91226200	2.83258400	-1.52640900
C	-0.53567600	3.05284400	-2.18625800
C	0.64096400	3.76079000	-1.35289300
C	1.98395200	2.91010800	-1.78525600
C	3.06326700	2.49965400	-0.74446700
C	3.94368700	1.11390900	-0.92033900
C	3.98739800	0.51537000	0.55507200
C	3.99778700	-1.02776200	0.81183400
C	3.08299300	-1.51199700	2.08855300
C	1.92119600	-2.11854700	1.40538500
C	0.68090000	-2.33491600	1.95359600
C	-0.34603300	-2.79111400	1.16134800
C	-1.64545200	-2.82971200	1.86234700
C	-2.82866800	-2.52050200	0.86393900
C	-3.43111800	-1.05084100	0.91750600
C	-2.57032500	-1.34088100	-1.26833600
C	-2.49274200	-2.72805400	-0.72228800
C	-1.16570400	-3.41590000	-1.13931000
C	-0.12562600	-3.05823400	-0.16174000
C	1.11461300	-2.85276000	-0.71104500
C	2.12459600	-2.34108600	0.06694000
C	3.47481700	-1.94369800	-0.38245700
C	3.43619000	-1.43442800	-1.85821500
C	3.43234400	0.14871000	-2.04270400
C	2.02380200	0.44102700	-2.37770500
C	1.38754600	1.65416200	-2.28407300
C	0.03495800	1.73358700	-2.50328500
C	-0.68095400	0.61405100	-2.84204600
C	-2.15733200	0.49976100	-2.94619100
C	-2.32810500	-1.06201900	-2.70839100
C	-0.97659500	-1.70672000	-3.19475000

C	-0.46600100	-3.03092900	-2.53288400
C	1.14900500	-3.02895400	-2.17711300
C	2.11103800	-1.92582400	-2.71538700
C	1.32099700	-0.67657900	-2.75581400
C	-0.03235700	-0.59284600	-2.96945000
C	-2.58613300	1.69098200	0.42527700
C	-1.78370100	2.63396500	-0.04815500
C	-1.03117300	3.60348200	0.78459600
C	0.40412100	3.87495400	0.19767800
C	1.20624100	2.87914300	0.95075800
C	2.35229700	2.24266100	0.52857100
C	2.83812600	1.16304600	1.22560100
C	2.22677100	0.75764700	2.39056300
C	2.50891300	-0.50194700	3.12036800
C	1.06288900	-0.78271400	3.87062600
C	0.22673600	-1.99458500	3.31918700
C	-1.33315200	-1.87229200	3.07179900
C	-1.70394800	-0.47965800	2.72278300
C	-3.03253700	-0.15633500	2.12627900
C	-2.90170900	1.38574600	1.85053100
C	-1.77146600	1.89234100	2.79684300
C	-0.80632100	3.02435400	2.23346100
C	0.56922700	2.45956700	2.09780000
C	1.09578600	1.40841700	2.82183600
C	0.30155700	0.60465700	3.78326700
C	-1.04357300	0.59705900	3.13068200
F	-4.66237900	1.24868400	-0.45064800
F	-3.88442400	2.09260600	-2.65634600
F	-2.63916700	3.96877900	-1.71789100
F	-0.72336100	3.76959200	-3.32861100
F	0.77973600	5.00866200	-1.83138900
F	2.57663800	3.60057300	-2.79336700
F	3.95519800	3.51347400	-0.60304400
F	5.20015500	1.46800800	-1.24530000
F	5.11753300	1.01506200	1.13892100
F	5.27221900	-1.38055100	1.05992900
F	3.80210200	-2.45601700	2.74854900
F	-1.84939500	-4.07911200	2.36643300
F	-3.82315300	-3.37273200	1.17535000
F	-4.78978600	-1.15843400	0.93508300
F	-3.50863100	-3.45161200	-1.26626900
F	-1.36584500	-4.76260200	-1.13591000
F	4.25474500	-3.06486700	-0.37461000
F	4.53074100	-1.91226400	-2.47655200

F	4.18330200	0.40828300	-3.15419900
F	-2.55828300	0.76984000	-4.21910400
F	-3.32146500	-1.60120100	-3.45543300
F	-1.08911300	-1.93254500	-4.53476100
F	-0.69365600	-4.03390700	-3.39725300
F	1.62678400	-4.25246700	-2.51958900
F	2.55099900	-2.27190400	-3.95138200
F	-1.73122200	4.76352900	0.83219200
F	0.76658100	5.12983100	0.58581800
F	3.42661700	-0.30074400	4.09988200
F	1.32309600	-1.02253100	5.16794200
F	0.43098200	-3.05247600	4.15176400
F	-2.03426300	-2.25506200	4.16653700
F	-3.96690900	-0.34341200	3.10202700
F	-4.07187700	2.00278700	2.15484500
F	-2.34994200	2.35925400	3.93251500
F	-0.81906900	4.06650400	3.10394500
F	0.21514500	1.17208100	5.01753500
H	-5.87434800	0.46779000	-2.33621600
O	-5.31557700	-0.31532400	-2.41579300
H	-5.43119000	-0.61205200	-3.32700300
TS	imaginary vibrational frequency		-811.79 cm ⁻¹
C	-3.42506900	-0.27638800	-0.82651800
C	-3.31234400	1.24052900	-0.78414500
C	-2.60823300	1.93843200	-2.01484900
C	-1.68781600	3.07320900	-1.32149800
C	-0.25744500	3.33468700	-1.85331600
C	0.87316600	3.87412000	-0.84329200
C	2.22101400	3.03103800	-1.28192900
C	3.19791700	2.44566400	-0.22525000
C	4.03683200	1.05581200	-0.51180100
C	3.95008500	0.28079800	0.87787800
C	3.88952800	-1.28082000	0.94136600
C	2.86753500	-1.88312900	2.07985200
C	1.74539700	-2.36350600	1.24737200
C	0.46105900	-2.60284700	1.67576900
C	-0.51591500	-2.92403800	0.76337000
C	-1.87379200	-2.95907000	1.35543100
C	-2.96504200	-2.47352100	0.30911700
C	-3.64717300	-1.02474000	0.52345100
C	-2.29800500	-0.96014500	-1.44643400
C	-2.44653200	-2.41172200	-1.20512100
C	-1.18671800	-3.17566900	-1.64168000
C	-0.19955700	-3.03620600	-0.56214500

C	1.07885800	-2.79667200	-0.99617100
C	2.04247300	-2.42378800	-0.09132200
C	3.43086000	-2.02108700	-0.39266700
C	3.51402400	-1.33140300	-1.79293200
C	3.57980900	0.25851500	-1.78043100
C	2.21996200	0.65772300	-2.19633600
C	1.63220800	1.88211300	-2.00030700
C	0.30914800	2.05844500	-2.32493000
C	-0.40506800	1.03135800	-2.87481800
C	-1.88054800	0.95896500	-2.99909900
C	-2.02120200	-0.55475500	-2.75197400
C	-0.82192100	-1.24038100	-3.44233800
C	-0.37672500	-2.65054100	-2.92236400
C	1.20615500	-2.76659700	-2.46744400
C	2.24620100	-1.65611300	-2.80176100
C	1.51358800	-0.37060400	-2.78172900
C	0.19348400	-0.19109000	-3.11509900
C	-2.52828200	1.68901000	0.39889800
C	-1.66875400	2.65906600	0.11503900
C	-0.96827900	3.50020700	1.11836700
C	0.51289900	3.80030000	0.68537200
C	1.22980000	2.69497600	1.36788200
C	2.38470700	2.06974200	0.95355900
C	2.77599400	0.89066200	1.54040600
C	2.06319400	0.36897300	2.59629200
C	2.24685600	-0.98138100	3.18135600
C	0.73943800	-1.29176500	3.78293000
C	-0.09151300	-2.39173700	3.03160700
C	-1.61929500	-2.16507100	2.67890700
C	-1.91523300	-0.73136100	2.45812600
C	-3.19700700	-0.27044400	1.83377800
C	-2.97270700	1.26966600	1.75433900
C	-1.91055900	1.60808900	2.83997000
C	-0.87306000	2.75638700	2.49952200
C	0.49234900	2.16221900	2.40278900
C	0.92316600	1.00672200	3.02248300
C	0.02904800	0.12304900	3.80989600
C	-1.25692800	0.25379200	3.05765600
F	-4.56521300	1.77077200	-0.64712700
F	-3.56728500	2.56563800	-2.72464800
F	-2.36870600	4.25035900	-1.40050700
F	-0.34841300	4.21890500	-2.88434800
F	1.09363200	5.16697600	-1.13706700
F	2.91646500	3.82919400	-2.13352600

F	4.11411900	3.39282700	0.10420200
F	5.32637300	1.39113300	-0.70274200
F	5.04973500	0.65822100	1.59603700
F	5.13016600	-1.71141900	1.23489500
F	3.51205700	-2.92256500	2.67165300
F	-2.18188700	-4.24237100	1.69524900
F	-3.97238400	-3.37099900	0.38290900
F	-4.99298300	-1.22681700	0.65145600
F	-3.49304800	-2.95083400	-1.95247900
F	-1.49452300	-4.48647700	-1.84690700
F	4.17848300	-3.16237500	-0.47267900
F	4.63514700	-1.77614400	-2.38938600
F	4.43016100	0.61139400	-2.79071200
F	-2.24556900	1.27440300	-4.27012500
F	-3.43259600	-0.88786600	-3.67836100
F	-1.00768600	-1.30693000	-4.78671100
F	-0.57316600	-3.52721800	-3.92207700
F	1.66200900	-3.95363000	-2.94626100
F	2.77782600	-1.89857400	-4.02713600
F	-1.65331300	4.66339800	1.24939300
F	0.86589300	4.98547500	1.25727600
F	3.09148800	-0.93431800	4.24382200
F	0.88906200	-1.69341800	5.05770900
F	-0.00554500	-3.54287100	3.75491300
F	-2.42063700	-2.62997000	3.66993100
F	-4.17353700	-0.50517900	2.76036500
F	-4.13338000	1.91692400	2.03568500
F	-2.56543200	1.95722800	3.97692600
F	-0.93236500	3.69294000	3.48051900
F	-0.14522000	0.53749900	5.09523400
H	-4.21763700	-0.78497600	-2.74238300
O	-4.64790900	-0.50393100	-1.71217900
H	-5.25279300	-1.16943800	-1.32702000
IP			
C	-3.47498400	-0.19316400	-1.39183800
C	-3.24507700	1.30308700	-1.10953100
C	-2.39621700	2.14717800	-2.14153900
C	-1.59311400	3.18478200	-1.20364300
C	-0.11790300	3.53478600	-1.52098100
C	0.86062100	3.94244900	-0.31059800
C	2.27338000	3.17233100	-0.67264600
C	3.11214800	2.45724500	0.42249400
C	4.01206000	1.12368600	0.08004600
C	3.76584000	0.17712400	1.34103000

C	3.72671900	-1.37919300	1.20197800
C	2.57730600	-2.11919400	2.12059300
C	1.56921500	-2.47480900	1.09964100
C	0.24491100	-2.76279900	1.32579700
C	-0.61035500	-2.94764700	0.26452600
C	-2.02334900	-3.10589700	0.67181800
C	-3.00843800	-2.52024800	-0.42954200
C	-3.73727400	-1.10708200	-0.11265100
C	-2.33751800	-0.85077300	-2.09097200
C	-2.34760400	-2.32860300	-1.90833400
C	-0.95445500	-2.94207200	-2.22874400
C	-0.13212800	-2.87687000	-1.01280100
C	1.18997000	-2.59169400	-1.24191900
C	2.03094900	-2.35308700	-0.18640300
C	3.44516100	-1.93939300	-0.26145100
C	3.70334500	-1.08445700	-1.54487600
C	3.74546300	0.49295900	-1.33062100
C	2.45331300	0.94813400	-1.88882500
C	1.81562800	2.13302500	-1.61896500
C	0.54446500	2.35098600	-2.10173000
C	-0.06560200	1.40994800	-2.88427300
C	-1.53451100	1.28787200	-3.12250900
C	-1.59669900	-0.22151900	-2.98535600
C	-0.37664000	-0.80263000	-3.67973200
C	0.02245100	-2.26162100	-3.31293100
C	1.51989500	-2.42096600	-2.66805500
C	2.58715400	-1.28509300	-2.74877200
C	1.85603600	0.00320400	-2.69744000
C	0.59562500	0.22671200	-3.19334400
C	-2.61077300	1.58804200	0.20787800
C	-1.74283200	2.59213100	0.16038700
C	-1.20451200	3.31490600	1.34182800
C	0.31078800	3.67796000	1.13995500
C	0.95515400	2.49753200	1.76652000
C	2.16103100	1.92952600	1.42563100
C	2.50243200	0.69241800	1.91570300
C	1.67673200	0.04530900	2.80788200
C	1.80929600	-1.36691900	3.24141900
C	0.24139100	-1.75497400	3.60238800
C	-0.47123000	-2.75193200	2.61842400
C	-1.95321500	-2.49631100	2.11438200
C	-2.24673800	-1.04680600	2.04340700
C	-3.44483800	-0.51036700	1.32138900
C	-3.22212400	1.02378600	1.44037700

C	-2.31825600	1.23056500	2.68878400
C	-1.26900400	2.41398200	2.62552000
C	0.10797200	1.84139700	2.63329400
C	0.48033400	0.62170900	3.16130700
C	-0.49062400	-0.35568500	3.71392400
C	-1.67466200	-0.13897500	2.82603500
F	-4.50029600	1.86495100	-1.05080100
F	-3.25302900	2.86391100	-2.89366300
F	-2.29016100	4.35591000	-1.21449000
F	-0.11594700	4.55701800	-2.41952700
F	1.08733400	5.26305900	-0.41029300
F	3.05796300	4.08221800	-1.30698200
F	3.95170500	3.35990800	0.99408300
F	5.30646400	1.48956400	0.10603900
F	4.75741700	0.46340200	2.23614500
F	4.92708300	-1.84632800	1.58984600
F	3.15289600	-3.22998200	2.64805100
F	-2.30215700	-4.43370100	0.80007000
F	-3.99520800	-3.42751900	-0.55587800
F	-5.07313800	-1.34961500	-0.11446300
F	-3.23548200	-2.86226200	-2.79300900
F	-1.14000300	-4.23863800	-2.59989100
F	4.19599900	-3.07389500	-0.38983500
F	4.89966700	-1.45807800	-2.03434300
F	4.72562600	0.96313600	-2.15906400
F	-1.84586400	1.64638700	-4.40260000
F	-0.52900700	-0.71935300	-5.03355400
F	-0.02194800	-2.99992500	-4.43449400
F	2.05199000	-3.56080500	-3.18195400
F	3.28019200	-1.40908000	-3.90850900
F	-1.93365000	4.44329000	1.52183300
F	0.56584000	4.78419400	1.89307500
F	2.51059200	-1.45801000	4.39958800
F	0.23871900	-2.31557900	4.82414800
F	-0.43908500	-3.99044100	3.18246800
F	-2.85277600	-3.09919000	2.92929100
F	-4.52095700	-0.82060800	2.10638800
F	-4.41277500	1.64837700	1.63670400
F	-3.12198800	1.43578300	3.76353400
F	-1.46977800	3.22745600	3.69376300
F	-0.83293700	-0.10569800	5.00794600
O	-4.52966100	-0.33245000	-2.29290800
H	-5.34903400	-0.03305200	-1.86336000

C₁-S_N2'-C19-F_f

RC

C	-3.06929500	-0.36335700	-0.47553100
C	-3.26838800	1.05676100	-0.84778500
C	-2.70040900	1.49943200	-2.23667800
C	-1.74576200	2.76873500	-1.85033200
C	-0.33560600	2.87397500	-2.47321200
C	0.84604700	3.60625200	-1.66583800
C	2.16424000	2.66593700	-1.97411300
C	3.19772900	2.30963400	-0.86776200
C	4.01896200	0.87769500	-0.89249000
C	3.99723900	0.41314600	0.63121100
C	3.92923300	-1.10221700	1.02334900
C	2.95344900	-1.43134600	2.30250000
C	1.78719700	-2.04398100	1.63270600
C	0.52422800	-2.16006800	2.15696600
C	-0.49628700	-2.65241200	1.37935400
C	-1.81537000	-2.57454700	2.04073200
C	-2.95273500	-2.30835200	0.97937100
C	-3.49471900	-0.81661300	0.88667300
C	-2.55985500	-1.32502600	-1.22878900
C	-2.57426400	-2.66113700	-0.56899800
C	-1.27545500	-3.44738700	-0.88284000
C	-0.24814500	-3.04841800	0.09364300
C	1.01555000	-2.94364600	-0.43159400
C	2.02364300	-2.40185200	0.32900500
C	3.40433000	-2.10150600	-0.10342600
C	3.43162300	-1.72448200	-1.61670100
C	3.49586100	-0.16519000	-1.93606200
C	2.10910900	0.14967400	-2.32897500
C	1.52805700	1.39302900	-2.36923100
C	0.18863800	1.50850400	-2.64103400
C	-0.56183500	0.39188300	-2.90008100
C	-2.03275700	0.33040500	-3.05447600
C	-2.28256000	-1.18677300	-2.68375000
C	-0.95467700	-1.93541000	-3.07316200
C	-0.52095800	-3.21664700	-2.28246100
C	1.08425300	-3.25045400	-1.87522800
C	2.11151700	-2.23783600	-2.47086800
C	1.37403400	-0.96734600	-2.63978300
C	0.03298400	-0.84811800	-2.90528100
C	-2.51994500	1.83465800	0.17484400
C	-1.66787200	2.70093600	-0.35481000
C	-0.89618100	3.70679000	0.41576900
C	0.56687100	3.86564100	-0.14196600

C	1.30383100	2.90774800	0.72036600
C	2.44202600	2.20013600	0.40080100
C	2.86193400	1.16972800	1.20796300
C	2.19365200	0.88941700	2.37887500
C	2.39669200	-0.31218300	3.22383000
C	0.91787900	-0.46703500	3.94619800
C	0.04782400	-1.68656200	3.47377600
C	-1.49863900	-1.52631200	3.17326700
C	-1.80720500	-0.15496400	2.69877600
C	-3.09885400	0.17007700	2.02359400
C	-2.88844500	1.67164100	1.60937500
C	-1.76908700	2.21565500	2.54761900
C	-0.73800800	3.24885000	1.91690200
C	0.61226500	2.61380100	1.87450900
C	1.07283800	1.61437500	2.70755100
C	0.21909300	0.93636100	3.71355400
C	-1.11040400	0.92662000	3.02734300
F	-4.58947700	1.38756300	-0.74019800
F	-3.72181300	1.97408700	-2.97002300
F	-2.42449800	3.90309400	-2.17227700
F	-0.44691000	3.48474500	-3.68451400
F	1.05369900	4.80093900	-2.24458800
F	2.81150100	3.23285800	-3.02449500
F	4.13183400	3.29165100	-0.79310100
F	5.29775000	1.14808700	-1.21037500
F	5.13569300	0.91039300	1.19921200
F	5.17775800	-1.48372400	1.34830600
F	3.60451100	-2.34649800	3.06635600
F	-2.08758300	-3.76582100	2.64334400
F	-3.99158400	-3.09334100	1.32237500
F	-4.86040600	-0.87348600	0.88177100
F	-3.61973900	-3.36978600	-1.08938900
F	-1.53972400	-4.77806600	-0.76894600
F	4.13431300	-3.24914000	0.02757600
F	4.52307700	-2.29482200	-2.15564200
F	4.27850500	-0.03418500	-3.04830900
F	-2.36481900	0.49602100	-4.36396000
F	-3.29966700	-1.72146800	-3.39772300
F	-1.03844300	-2.26895700	-4.39149100
F	-0.76790900	-4.28277900	-3.06129100
F	1.51439700	-4.51819800	-2.09680100
F	2.57489400	-2.70605300	-3.65660700
F	-1.54524600	4.89436600	0.33757900
F	0.97304800	5.13333400	0.14878100

F	3.29224300	-0.06793600	4.21312800
F	1.12967400	-0.60214500	5.26723100
F	0.18322000	-2.67821800	4.39674000
F	-2.23432700	-1.79237500	4.28001800
F	-4.08111300	0.12655200	2.96890000
F	-4.04071400	2.36044500	1.81240600
F	-2.36698700	2.81184500	3.60946200
F	-0.72538700	4.36388500	2.69173400
F	0.12937400	1.61879000	4.88816600
H	-5.56877600	-1.77169000	-2.10088700
O	-5.49848100	-0.81114200	-2.02893500
H	-6.05034700	-0.58200400	-1.27080100
TS	imaginary vibrational frequency		-872.35 cm ⁻¹
C	-2.73256600	-0.29058700	-0.44132000
C	-2.95910600	0.95559400	-1.03968300
C	-2.54616400	1.27440600	-2.48426200
C	-1.58232200	2.57695300	-2.28245600
C	-0.15366700	2.50387900	-2.86335900
C	1.04255700	3.28999100	-2.15198700
C	2.31633600	2.24959300	-2.28986500
C	3.30744900	2.00655100	-1.12019600
C	4.05414300	0.54694600	-0.91524600
C	3.97863500	0.31541500	0.65764700
C	3.82483900	-1.12080000	1.26460900
C	2.81623000	-1.20743000	2.55488800
C	1.62924000	-1.85111500	1.95573000
C	0.35477900	-1.82301300	2.46134500
C	-0.68040400	-2.34702000	1.72566100
C	-1.99515100	-2.13119800	2.34420900
C	-3.09803700	-1.95902900	1.23993300
C	-3.39935700	-0.47695300	0.87887600
C	-3.03086400	-1.46244200	-1.24681900
C	-2.83825000	-2.64207000	-0.25565200
C	-1.47780000	-3.41983700	-0.42537700
C	-0.45227200	-2.90288200	0.50016200
C	0.82809300	-2.97387500	0.01321700
C	1.86002100	-2.40323600	0.72056400
C	3.26379100	-2.24865500	0.28454900
C	3.33913100	-2.10527600	-1.26621900
C	3.49930100	-0.61413400	-1.81144400
C	2.13941700	-0.29066400	-2.28511600
C	1.62246900	0.96267300	-2.50620100
C	0.29430800	1.10313900	-2.81040300
C	-0.50828800	-0.00311200	-2.91690900

C	-1.96293800	-0.00452100	-3.14711400
C	-2.37626500	-1.48345400	-2.65218400
C	-1.01910700	-2.30629700	-2.78001300
C	-0.68277100	-3.46569000	-1.80555200
C	0.91084400	-3.51931100	-1.35570800
C	2.00770900	-2.66975200	-2.06882700
C	1.34593100	-1.40143100	-2.43376700
C	0.01212600	-1.25232300	-2.71775500
C	-2.49714300	2.02795100	-0.16170800
C	-1.59346200	2.78294100	-0.79242200
C	-0.74454500	3.81693800	-0.14658900
C	0.74300000	3.78475400	-0.69309100
C	1.40956000	2.92070400	0.31218800
C	2.51683800	2.11923300	0.12663200
C	2.87287000	1.20241100	1.08567300
C	2.17650700	1.13668000	2.27167500
C	2.30575700	0.06491700	3.28855400
C	0.81335300	0.09350300	3.99578100
C	-0.11400500	-1.14114700	3.68769900
C	-1.64035500	-0.94440300	3.32781400
C	-1.84616300	0.36270700	2.65969100
C	-3.08667500	0.62140800	1.89502600
C	-2.85151900	2.05111200	1.29070000
C	-1.71099200	2.67898800	2.16040200
C	-0.61958600	3.55096300	1.40735400
C	0.69326500	2.84248100	1.48354900
C	1.09618200	1.96230000	2.46930600
C	0.19993500	1.48999700	3.55264700
C	-1.11596700	1.45199000	2.84954600
F	-4.68920800	0.99191800	-1.24147900
F	-3.58249200	1.68648500	-3.23737000
F	-2.19674800	3.64546300	-2.85727300
F	-0.20580200	2.91810400	-4.16037700
F	1.32149300	4.37322500	-2.89719400
F	3.00512800	2.62638600	-3.39801600
F	4.28987800	2.94297100	-1.15590200
F	5.35122300	0.70601800	-1.23721800
F	5.13027800	0.83426000	1.17950800
F	5.04707900	-1.51282700	1.66678100
F	3.40587300	-2.03105400	3.46020700
F	-2.32510000	-3.21480500	3.10324500
F	-4.21408400	-2.54318100	1.72791400
F	-4.79424400	-0.43718100	0.76184400
F	-3.83974300	-3.54174200	-0.46093400

F	-1.74339400	-4.71470600	-0.07889500
F	3.92673900	-3.39914700	0.60663200
F	4.40349600	-2.80969400	-1.68814600
F	4.31724900	-0.69093000	-2.90209400
F	-2.21646900	0.05280800	-4.48329700
F	-3.23646100	-2.02141100	-3.53974500
F	-1.00077100	-2.83088000	-4.04113200
F	-0.98329000	-4.62426000	-2.41581500
F	1.27021300	-4.82752400	-1.35673700
F	2.46356800	-3.33124900	-3.16217000
F	-1.27760100	5.04497300	-0.36887800
F	1.23401000	5.05121100	-0.57547400
F	3.20059000	0.41105100	4.24941000
F	1.00131400	0.13423900	5.32672400
F	-0.04187600	-1.98917900	4.75069500
F	-2.42142100	-1.00263400	4.43391800
F	-4.10520500	0.68890200	2.80293400
F	-3.98926300	2.78181100	1.41334500
F	-2.28981500	3.45934500	3.10871700
F	-0.54377900	4.75951000	2.02289800
F	0.14399100	2.34007300	4.61515300
H	-5.07171600	-1.95473900	-1.05606700
O	-4.52855800	-1.35473700	-1.60582400
H	-4.79127900	-0.25725500	-1.43368900
IP			
C	-3.04928900	-0.09393300	-0.77923200
C	-2.57763000	0.94176800	-1.45386300
C	-2.18778000	0.96727600	-2.89339000
C	-1.12476900	2.20662300	-2.92305500
C	0.32595800	1.88915000	-3.33578100
C	1.53865600	2.68584600	-2.65735800
C	2.68531500	1.52106800	-2.44823900
C	3.53524000	1.43152600	-1.15371400
C	4.08885600	-0.01867400	-0.59037400
C	3.85281400	0.08433000	0.98075600
C	3.48555300	-1.17556200	1.83578200
C	2.36168700	-0.89944700	3.00161700
C	1.16541700	-1.52723100	2.40436900
C	-0.13748300	-1.26142800	2.73895300
C	-1.15902800	-1.80843400	2.00015100
C	-2.49561000	-1.37829500	2.44064900
C	-3.50151200	-1.35515600	1.22606800
C	-3.67942800	0.06073400	0.56437600
C	-3.27097000	-1.45154000	-1.34208700

C	-3.16338700	-2.37974700	-0.06462000
C	-1.86927300	-3.25834900	0.05844200
C	-0.88251500	-2.62272800	0.94255800
C	0.41782100	-2.92915500	0.63349900
C	1.44127800	-2.33676500	1.33099100
C	2.88642500	-2.42027500	1.03656600
C	3.11198100	-2.60471000	-0.49583000
C	3.48184500	-1.27831100	-1.29704000
C	2.21142700	-0.93143400	-1.96353200
C	1.86568800	0.29139600	-2.48526700
C	0.59976600	0.48700300	-2.96969100
C	-0.31301300	-0.54127200	-2.95683900
C	-1.74210000	-0.44335000	-3.31557600
C	-2.36246500	-1.75788900	-2.59885100
C	-1.09744300	-2.70751900	-2.41259500
C	-0.97645100	-3.66374000	-1.19582800
C	0.55525800	-3.76818100	-0.57248200
C	1.79842900	-3.19438400	-1.31472500
C	1.31601100	-1.97073300	-1.98766700
C	0.03778700	-1.76226500	-2.44762100
C	-2.15979000	2.13705800	-0.79433500
C	-1.20672600	2.73770700	-1.51230900
C	-0.33046400	3.81231000	-0.99777100
C	1.18298500	3.50581600	-1.36104100
C	1.64387600	2.80117000	-0.13821500
C	2.65796900	1.87109300	-0.04521200
C	2.81901800	1.13787800	1.10562100
C	2.01718500	1.38241000	2.19842900
C	1.93737300	0.53731700	3.41516500
C	0.39977100	0.85181500	3.93897100
C	-0.63139400	-0.32439400	3.76888600
C	-2.09559500	-0.06407800	3.22410300
C	-2.09509000	1.09388600	2.29635600
C	-3.22668800	1.32016700	1.35897900
C	-2.71751100	2.54066400	0.52116000
C	-1.63026700	3.23977800	1.38070700
C	-0.38317800	3.84324500	0.59144300
C	0.82325300	3.03477300	0.94157700
C	1.02660000	2.33136300	2.11452400
C	-0.00674600	2.17714300	3.16961700
C	-1.25631700	2.12338600	2.35382700
F	-3.26785800	1.34098900	-3.62435100
F	-1.60098900	3.16360900	-3.76114000
F	0.43027800	2.04357600	-4.68446500

F	2.00512100	3.56008600	-3.56530100
F	3.50899200	1.58734800	-3.52609400
F	4.61693500	2.24442600	-1.26475200
F	5.41775600	-0.05537300	-0.79570900
F	5.00700100	0.58923300	1.50943800
F	4.61325000	-1.59124400	2.43900700
F	2.77047000	-1.57406000	4.10716000
F	-2.97492800	-2.27346000	3.35051000
F	-4.69391400	-1.74712400	1.71125800
F	-5.01687900	0.24157000	0.34020900
F	-4.19132600	-3.26040600	-0.13405500
F	-2.24451600	-4.43323300	0.65198000
F	3.37489400	-3.54088900	1.64591100
F	4.12305600	-3.47517300	-0.65625600
F	4.37130700	-1.65073400	-2.26431500
F	-1.91232500	-0.57862500	-4.65784700
F	-3.16506900	-2.38229800	-3.49451200
F	-1.01523900	-3.48380600	-3.53521000
F	-1.34974200	-4.89287700	-1.59201400
F	0.76401800	-5.07091500	-0.25902800
F	2.27041900	-4.10437100	-2.20218900
F	-0.68637400	5.01380600	-1.51123900
F	1.82314000	4.70565500	-1.44699900
F	2.78063300	0.98809000	4.37789800
F	0.46955600	1.14615400	5.24887400
F	-0.73570300	-0.96109600	4.96804500
F	-2.96021400	0.16752000	4.24007500
F	-4.29225800	1.73560900	2.10540100
F	-3.74565200	3.39182700	0.27327600
F	-2.21551100	4.24528200	2.07808100
F	-0.22630400	5.13464400	0.97988300
F	-0.05329100	3.22747300	4.03460900
O	-4.59782500	-1.42968900	-1.76815500
H	-4.85402800	-2.32375900	-2.05002800

C₁-S_N2'-C19-F_i

RC

C	-3.06929500	-0.36335700	-0.47553100
C	-3.26838800	1.05676100	-0.84778500
C	-2.70040900	1.49943200	-2.23667800
C	-1.74576200	2.76873500	-1.85033200
C	-0.33560600	2.87397500	-2.47321200
C	0.84604700	3.60625200	-1.66583800
C	2.16424000	2.66593700	-1.97411300
C	3.19772900	2.30963400	-0.86776200

C	4.01896200	0.87769500	-0.89249000
C	3.99723900	0.41314600	0.63121100
C	3.92923300	-1.10221700	1.02334900
C	2.95344900	-1.43134600	2.30250000
C	1.78719700	-2.04398100	1.63270600
C	0.52422800	-2.16006800	2.15696600
C	-0.49628700	-2.65241200	1.37935400
C	-1.81537000	-2.57454700	2.04073200
C	-2.95273500	-2.30835200	0.97937100
C	-3.49471900	-0.81661300	0.88667300
C	-2.55985500	-1.32502600	-1.22878900
C	-2.57426400	-2.66113700	-0.56899800
C	-1.27545500	-3.44738700	-0.88284000
C	-0.24814500	-3.04841800	0.09364300
C	1.01555000	-2.94364600	-0.43159400
C	2.02364300	-2.40185200	0.32900500
C	3.40433000	-2.10150600	-0.10342600
C	3.43162300	-1.72448200	-1.61670100
C	3.49586100	-0.16519000	-1.93606200
C	2.10910900	0.14967400	-2.32897500
C	1.52805700	1.39302900	-2.36923100
C	0.18863800	1.50850400	-2.64103400
C	-0.56183500	0.39188300	-2.90008100
C	-2.03275700	0.33040500	-3.05447600
C	-2.28256000	-1.18677300	-2.68375000
C	-0.95467700	-1.93541000	-3.07316200
C	-0.52095800	-3.21664700	-2.28246100
C	1.08425300	-3.25045400	-1.87522800
C	2.11151700	-2.23783600	-2.47086800
C	1.37403400	-0.96734600	-2.63978300
C	0.03298400	-0.84811800	-2.90528100
C	-2.51994500	1.83465800	0.17484400
C	-1.66787200	2.70093600	-0.35481000
C	-0.89618100	3.70679000	0.41576900
C	0.56687100	3.86564100	-0.14196600
C	1.30383100	2.90774800	0.72036600
C	2.44202600	2.20013600	0.40080100
C	2.86193400	1.16972800	1.20796300
C	2.19365200	0.88941700	2.37887500
C	2.39669200	-0.31218300	3.22383000
C	0.91787900	-0.46703500	3.94619800
C	0.04782400	-1.68656200	3.47377600
C	-1.49863900	-1.52631200	3.17326700
C	-1.80720500	-0.15496400	2.69877600

C	-3.09885400	0.17007700	2.02359400
C	-2.88844500	1.67164100	1.60937500
C	-1.76908700	2.21565500	2.54761900
C	-0.73800800	3.24885000	1.91690200
C	0.61226500	2.61380100	1.87450900
C	1.07283800	1.61437500	2.70755100
C	0.21909300	0.93636100	3.71355400
C	-1.11040400	0.92662000	3.02734300
F	-4.58947700	1.38756300	-0.74019800
F	-3.72181300	1.97408700	-2.97002300
F	-2.42449800	3.90309400	-2.17227700
F	-0.44691000	3.48474500	-3.68451400
F	1.05369900	4.80093900	-2.24458800
F	2.81150100	3.23285800	-3.02449500
F	4.13183400	3.29165100	-0.79310100
F	5.29775000	1.14808700	-1.21037500
F	5.13569300	0.91039300	1.19921200
F	5.17775800	-1.48372400	1.34830600
F	3.60451100	-2.34649800	3.06635600
F	-2.08758300	-3.76582100	2.64334400
F	-3.99158400	-3.09334100	1.32237500
F	-4.86040600	-0.87348600	0.88177100
F	-3.61973900	-3.36978600	-1.08938900
F	-1.53972400	-4.77806600	-0.76894600
F	4.13431300	-3.24914000	0.02757600
F	4.52307700	-2.29482200	-2.15564200
F	4.27850500	-0.03418500	-3.04830900
F	-2.36481900	0.49602100	-4.36396000
F	-3.29966700	-1.72146800	-3.39772300
F	-1.03844300	-2.26895700	-4.39149100
F	-0.76790900	-4.28277900	-3.06129100
F	1.51439700	-4.51819800	-2.09680100
F	2.57489400	-2.70605300	-3.65660700
F	-1.54524600	4.89436600	0.33757900
F	0.97304800	5.13333400	0.14878100
F	3.29224300	-0.06793600	4.21312800
F	1.12967400	-0.60214500	5.26723100
F	0.18322000	-2.67821800	4.39674000
F	-2.23432700	-1.79237500	4.28001800
F	-4.08111300	0.12655200	2.96890000
F	-4.04071400	2.36044500	1.81240600
F	-2.36698700	2.81184500	3.60946200
F	-0.72538700	4.36388500	2.69173400
F	0.12937400	1.61879000	4.88816600

H	-5.56877600	-1.77169000	-2.10088700
O	-5.49848100	-0.81114200	-2.02893500
H	-6.05034700	-0.58200400	-1.27080100
TS	imaginary vibrational frequency		-761.68 cm ⁻¹
C	-2.76980700	-0.25330600	-0.48655800
C	-3.08715200	1.11504200	-0.96487800
C	-2.55870200	1.50495400	-2.36978800
C	-1.57261600	2.76750800	-2.06387400
C	-0.14743500	2.73784500	-2.64911900
C	1.05375100	3.46011900	-1.87191400
C	2.32088700	2.42851200	-2.09031100
C	3.31299100	2.09199900	-0.94282700
C	4.05478200	0.61940000	-0.85908800
C	3.97897900	0.25887500	0.68949800
C	3.83027100	-1.22193800	1.17665300
C	2.81774800	-1.41726100	2.45617500
C	1.63611200	-2.01384800	1.80154400
C	0.35758300	-2.01441000	2.29898600
C	-0.67203800	-2.47686200	1.51986500
C	-1.99027100	-2.31945900	2.14928000
C	-3.08478100	-2.05594500	1.05699500
C	-3.28927700	-0.55670000	0.78308800
C	-3.03485900	-1.38241900	-1.35511300
C	-2.81704000	-2.64515900	-0.46412600
C	-1.45315100	-3.38806900	-0.70146800
C	-0.43334500	-2.94254800	0.25993000
C	0.84593900	-2.97843000	-0.22904000
C	1.87492300	-2.46934700	0.52850700
C	3.27624400	-2.26883700	0.10491000
C	3.34242200	-1.99019900	-1.43092100
C	3.49398300	-0.46046100	-1.84686200
C	2.13122200	-0.10058200	-2.28354600
C	1.61941000	1.16677200	-2.40472100
C	0.29157600	1.33428300	-2.69387600
C	-0.51729200	0.24301900	-2.87929600
C	-1.97098900	0.26871700	-3.11231700
C	-2.39507200	-1.25166700	-2.74945400
C	-1.03336500	-2.06515200	-2.95282400
C	-0.67781300	-3.30635600	-2.08615800
C	0.92125500	-3.39993300	-1.64370200
C	2.00949800	-2.48613300	-2.27792800
C	1.33614000	-1.19409100	-2.52252200
C	-0.00027000	-1.02051200	-2.79048600
C	-2.44162200	2.02351000	0.00028900

C	-1.54624400	2.82285300	-0.56474300
C	-0.72347800	3.81383500	0.16553600
C	0.76023100	3.83599800	-0.37333900
C	1.42033100	2.89016500	0.56022500
C	2.52469200	2.10398700	0.31126800
C	2.86983400	1.10369100	1.18789200
C	2.16626400	0.93738600	2.35982100
C	2.29654100	-0.21034400	3.28852500
C	0.79929400	-0.24019800	3.99020900
C	-0.12247600	-1.44059000	3.57497300
C	-1.65669800	-1.22291800	3.23631600
C	-1.89554900	0.14032800	2.69276800
C	-3.12515600	0.46478000	1.90071700
C	-2.84262900	1.94049600	1.43281200
C	-1.72028100	2.48894500	2.36671200
C	-0.61855600	3.41973900	1.69249200
C	0.69042300	2.70383000	1.71191600
C	1.08046700	1.73945800	2.61846100
C	0.17884600	1.18217600	3.65647700
C	-1.14546100	1.20375500	2.95867900
F	-4.46031900	1.34320800	-0.97038100
F	-3.58538200	1.96743400	-3.11690100
F	-2.18206400	3.89450900	-2.52466700
F	-0.18900300	3.24817900	-3.91170400
F	1.33839800	4.59917200	-2.52610100
F	3.01299700	2.88171400	-3.16791800
F	4.29679500	3.02685900	-0.90743500
F	5.35229700	0.79859200	-1.16808900
F	5.12910000	0.73808900	1.25091200
F	5.05261500	-1.64042200	1.55086600
F	3.41033900	-2.30716200	3.29388400
F	-2.31802900	-3.47019900	2.80137700
F	-4.20557600	-2.64610500	1.51681300
F	-4.99396200	-0.57387600	0.57436200
F	-3.78256300	-3.55548100	-0.71064000
F	-1.69002500	-4.71327400	-0.46820900
F	3.95176000	-3.43610700	0.32175100
F	4.40819800	-2.65009000	-1.91636500
F	4.30170300	-0.44075400	-2.94822600
F	-2.21008700	0.42300400	-4.44613100
F	-3.28270400	-1.68164500	-3.68125200
F	-1.02696900	-2.46769700	-4.25714800
F	-0.97767600	-4.40663800	-2.79588700
F	1.27868200	-4.70219600	-1.76617400

F	2.46585500	-3.03925800	-3.42956600
F	-1.27316400	5.04650800	0.03062500
F	1.25317800	5.08838700	-0.15836300
F	3.18569200	0.06183500	4.27715700
F	0.98172400	-0.30509300	5.32088400
F	-0.05379900	-2.37863900	4.55986200
F	-2.41863400	-1.40886500	4.34130600
F	-4.19956600	0.44587500	2.73209700
F	-3.97503300	2.67640000	1.57653500
F	-2.30869100	3.19522000	3.36556400
F	-0.54381000	4.57048800	2.41135100
F	0.12364000	1.94651600	4.78282300
H	-4.97998200	-1.01786700	-0.64239400
O	-4.58256100	-1.42370600	-1.59586000
H	-4.84803300	-0.85871300	-2.34814500
IP			
C	-3.08573600	-0.46837800	-0.31936300
C	-3.39142300	0.91053100	-0.78798800
C	-2.91762600	1.25553600	-2.23094300
C	-1.97310700	2.57641000	-2.00686200
C	-0.58950000	2.63075400	-2.68398200
C	0.61037500	3.45435600	-2.00563600
C	1.93073800	2.50749900	-2.28347200
C	3.02117000	2.27091600	-1.19807400
C	3.86749000	0.85405300	-1.12815000
C	3.92133800	0.53316900	0.43121600
C	3.90137000	-0.94018900	0.96130000
C	2.99110200	-1.16634300	2.30985100
C	1.80919500	-1.85737900	1.75428500
C	0.57318700	-1.94631700	2.34586800
C	-0.46941800	-2.51899600	1.65837800
C	-1.76297400	-2.41450100	2.35576800
C	-2.87928600	-2.19085900	1.28839600
C	-3.00219500	-0.73177400	0.97783500
C	-3.20428500	-1.69079100	-1.16402800
C	-2.72077700	-2.85750800	-0.19995500
C	-1.33163800	-3.52342600	-0.50318200
C	-0.28499800	-2.99108100	0.38809000
C	0.95800300	-2.93998800	-0.18974500
C	1.99299400	-2.32830100	0.47777800
C	3.34769700	-2.04962000	-0.04347400
C	3.29993600	-1.81390600	-1.58611000
C	3.31760400	-0.28827000	-2.04712700
C	1.90542900	-0.03186300	-2.38868300

C	1.29709600	1.19319100	-2.51205800
C	-0.05635700	1.26074100	-2.70912900
C	-0.80273500	0.11332900	-2.78816000
C	-2.26635400	0.02673400	-2.96103600
C	-2.53891000	-1.52013900	-2.56597800
C	-1.13423200	-2.22800000	-2.80295100
C	-0.64967800	-3.42124400	-1.93393000
C	0.97398600	-3.39302500	-1.59695600
C	1.94868200	-2.41998900	-2.32259000
C	1.17374000	-1.18082400	-2.53626100
C	-0.18708600	-1.10449000	-2.69928400
C	-2.65515100	1.82851000	0.12440200
C	-1.83623200	2.64797500	-0.51664100
C	-1.04096400	3.71964000	0.13148600
C	0.39457500	3.84536200	-0.50017400
C	1.18680600	2.98260500	0.41229200
C	2.32512100	2.26822500	0.10877500
C	2.79748200	1.32220000	0.98728500
C	2.18656600	1.14122200	2.20877900
C	2.45143000	0.02535700	3.14953000
C	1.01097600	-0.08548000	3.95243900
C	0.14498800	-1.36239800	3.63724800
C	-1.42314100	-1.26149700	3.40732600
C	-1.78442500	0.08358000	2.87942700
C	-3.02081800	0.28257800	2.07459400
C	-2.91949900	1.76465300	1.58954500
C	-1.78543600	2.42250600	2.43478300
C	-0.80510200	3.40086200	1.66091100
C	0.55364000	2.78699700	1.61961200
C	1.06842200	1.87795600	2.52313100
C	0.28146600	1.28867900	3.63591400
C	-1.08726300	1.20255600	3.04267000
F	-4.73722000	1.12098500	-0.67804200
F	-3.98467400	1.64325000	-2.95313600
F	-2.67810300	3.66649400	-2.41346400
F	-0.74702000	3.09699000	-3.95344700
F	0.76872200	4.59256900	-2.70219400
F	2.51867400	2.97487500	-3.41428300
F	3.93953100	3.26871900	-1.25805100
F	5.12448100	1.11173400	-1.53170800
F	5.07378900	1.09953200	0.89870900
F	5.17173000	-1.26832000	1.25967400
F	3.69610300	-1.99438800	3.12361800
F	-2.03645000	-3.55315100	3.04670400

F	-4.04708800	-2.64787000	1.81058700
F	-3.63505900	-3.84875100	-0.30294000
F	-1.46230800	-4.85746300	-0.23391700
F	4.10679700	-3.16705000	0.15987200
F	4.37481300	-2.41507900	-2.12429500
F	4.04273200	-0.24427300	-3.20328300
F	-2.55591000	0.15186100	-4.28729200
F	-3.39515500	-2.05078400	-3.47635200
F	-1.11451500	-2.65638700	-4.10188700
F	-0.91969600	-4.55549200	-2.60292300
F	1.42050800	-4.66818400	-1.71231900
F	2.35567700	-2.96329000	-3.49712000
F	-1.70537000	4.89207100	-0.01959800
F	0.79295500	5.13927700	-0.34521500
F	3.38511100	0.37383600	4.07153800
F	1.28724700	-0.10129600	5.26808000
F	0.35226500	-2.25981500	4.64043000
F	-2.09420900	-1.48034600	4.56294000
F	-4.13553300	0.10777800	2.84301300
F	-4.09933300	2.39654900	1.81562100
F	-2.36332000	3.12639000	3.44166300
F	-0.77902500	4.58636000	2.32343500
F	0.26088200	2.07522900	4.74790700
O	-4.58451600	-1.78399400	-1.34071100
H	-4.77968500	-2.47373100	-1.99718700