

Structural variation in the ferrobustamite solid solution

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Abstract

Ferrobustamite, $\text{Wo}_{82}\text{Fs}_{18}$, from the Ofuku mine, Yamaguchi Prefecture, Japan, is close to the Fe-poor end of the ferrobustamite solid solution. Its crystal data are: space group $A\bar{1}$, $a = 7.862$, $b = 7.253$, $c = 13.967 \text{ \AA}$, $\alpha = 89^\circ 44'$, $\beta = 95^\circ 28'$, $\gamma = 103^\circ 29'$, and $12[\text{Ca}_{0.82}\text{Fe}_{0.15}\text{Mn}_{0.03}\text{SiO}_3]$ in the unit cell. Our refinement of its structure reveals that it possesses pseudo-mirrors which are more nearly true mirror planes than those in the $\text{Wo}_{50}\text{Fs}_{50}$ structure, and the small size of one cation site, $M3$, in the structure induces the concentration of the Fe(Mn) content into it, thus giving the solid solution the Fe-poor limit of $\text{Wo}_{83.3}\text{Fs}_{16.7}$. The Mössbauer spectra of the specimen showed that, after a heat treatment at $1,140^\circ\text{C}$, the degree of concentration of Fe at $M3$ decreases, suggesting that the site occupancies of Fe atoms vary with the temperature of formation and the cooling process of the crystal.

Introduction

Bowen *et al.* (1933) presented a phase diagram of the system $\text{CaO}-\text{FeO}-\text{SiO}_2$ showing an extensive solid solution at temperatures above $1,000^\circ\text{C}$, and called it the "wollastonite solid solution." Tilley (1937) first described a mineral with a composition of 77 mole percent CaSiO_3 and 23 percent FeSiO_3 ($\text{Wo}_{77}\text{Fs}_{23}$) from Scawt Hill, County, Antrim, and named it "iron-wollastonite." He further reported another iron-wollastonite from contact skarns at Skye, Scotland (Tilley, 1948).

A reexamination by Rutstein (1971) of the $\text{CaSiO}_3-\text{CaFeSiO}_6$ system showed that there are two different phases in this system, and these are compositionally separated from each other by a gap extending from $\text{Wo}_{88}\text{Fs}_{12}$ to $\text{Wo}_{78}\text{Fs}_{22}$. Rutstein and White (1971) analyzed infrared spectra of these samples, and suggested that those rich in iron have a structure analogous to that of bustamite.

The crystal structures of two pyroxenoids, a synthetic phase, $\text{Ca}_{0.5}\text{Fe}_{0.5}\text{SiO}_3$ ($\text{Wo}_{50}\text{Fs}_{50}$), and a natural phase, $\text{Ca}_{0.79}\text{Fe}_{0.19}\text{Mn}_{0.02}\text{SiO}_3$ ($\text{Wo}_{79}\text{Fs}_{21}$), both refined by Rapoport and Burnham (1973), are similar to each other and to that of bustamite. This species was therefore named ferrobustamite by these authors, who pointed out that the Fe-poor end-member of this phase region is expected on structural grounds to lie at $\text{Wo}_{5/6}\text{Fs}_{1/6}$.

From chemical analyses of natural samples,

Shimazaki and Yamanaka (1973) discovered a miscibility gap between wollastonite and ferrobustamite, and suggested that ferrobustamite with an Fe content larger than that of $\text{Ca}_{5/6}\text{Fe}_{1/6}\text{SiO}_3$ ($\text{Wo}_{83.3}\text{Fs}_{16.7}$) will be stable at the low temperatures appropriate for skarn formation, probably $300-600^\circ\text{C}$. Matsueda (1973, 1974) also reconfirmed that ferrobustamite is distinct from wollastonite in optical and chemical properties and cell dimensions, and considered paragenetic relations between ferrobustamite and wollastonite. Compositional limits of wollastonite, bustamite, and ferrobustamite were also discussed by Mason (1975).

Since the structure refinement of the natural phase, $\text{Wo}_{79}\text{Fs}_{21}$, reported by Rapoport and Burnham (1973), was hindered by the twinned crystal used for the structure determination, we consider it necessary to reexamine the structure with a well-specified crystal. Also the structure of ferrobustamite in the Fe-poor limit was of particular importance for clarifying structure variations of the solid solution. We have therefore undertaken a structural investigation of $\text{Ca}_{0.82}\text{Fe}_{0.15}\text{Mn}_{0.03}\text{SiO}_3$ and compared our results with the data previously obtained from other members of the series.

Refinement of the ferrobustamite structure

The crystal used in the present investigation was found in the Ofuku mine, Yamaguchi Prefecture,

-1	7	-6	-7	41	-42	0	20	20	-6	35	-36	-3	13	-13	H,L = 5-13					
H,L = -6-15	-5	11	-10	H,L = -2-14	-4	24	23	-1	13	13	-7	19	20	H,L = -4-12						
-3	26	-27	-3	11	-10	-8	-2	-2	23	23	-3	10	-8	-6	28	28				
-1	17	17	-1	9	9	-6	26	27	0	33	-5	22	-24	-4	105	105				
H,L = -5-15	H,L = 5-15	-4	31	-30	H,L = 6-14	-1	11	11	-5	21	22	-2	5	4	H,L = -3-12					
-5	22	-22	-7	9	-8	-2	4	3	-8	29	-31	-1	27	28	-8	67	68			
-3	29	28	-5	31	-32	0	29	-29	-6	16	-16	-7	9	-9	H,L = 7-13					
-1	16	-16	-3	7	8	H,L = -1-14	-4	27	-27	-5	31	-31	-1	8	7	-6	10	-10		
H,L = -4-15	H,L = 6-15	-1	21	-20	-8	39	41	-2	19	21	H,L = -1-13	-1	11	-9	-4	14	15			
-5	15	18	-3	9	-8	-4	43	43	H,L = 7-14	-5	8	6	H,L = 8-15	H,L = -2-12						
-1	27	26	-1	12	13	-2	42	-41	-6	20	-19	-7	15	15	-6	79	-81			
H,L = -3-15	H,L = 7-15	0	31	30	-4	23	-23	-3	32	-33	-5	24	-24	-4	4	-5				
-5	7	-6	-7	31	33	H,L = 0-14	-2	40	-40	-1	29	28	-3	13	-13	-2	18	-17		
H,L = -2-15	-5	13	14	-8	37	-39	0	31	31	H,L = 0-15	-1	15	-14	0	150	153				
-7	8	-8	-1	18	19	-6	41	41	H,L = 8-14	-7	45	46	H,L = 9-13	H,L = -1-12						
-1	7	-6	-5	14	13	-4	13	-13	-6	22	22	-5	5	0	-6	35	35			
-3	21	21	-5	11	10	-2	32	81	-4	32	-32	-3	14	15	-1	13	13			
-1	7	-6	-3	24	25	0	37	-35	-2	25	-26	-1	22	-21	H,L = 10-13					
-5	14	13	H,L = 8-15	-1	18	-18	H,L = 1-14	0	54	-56	H,L = 1-13	-5	7	-5	0	47	-46			
-3	21	21	-5	11	10	-2	32	81	H,L = 9-14	-9	18	-18	-3	15	17	H,L = 0-12				
-1	7	-6	-3	24	25	-1	18	-18	H,L = 9-14	-6	17	18	-7	22	-22	-8	61	64		
H,L = -1-15	-1	18	-18	H,L = 1-14	0	54	-56	H,L = 1-14	-4	41	41	-5	28	29	H,L = -9-12					
-7	37	-38	H,L = 9-15	-6	78	-81	H,L = 9-14	-2	11	-11	-3	31	-31	-2	48	49	-4	112	-115	
-5	8	-9	-1	5	-6	-4	20	20	H,L = 10-14	-6	17	18	-7	22	-22	-1	13	14		
-3	17	16	H,L = -8-14	-2	38	-37	-4	41	41	H,L = 10-14	-1	32	32	0	56	-58	0	91	-90	
-1	24	23	-1	18	-18	H,L = -7-14	0	98	96	H,L = 10-14	-2	11	-11	-3	31	-31	-2	48	49	
-7	37	-38	H,L = -7-14	-6	78	-81	H,L = -7-14	-4	41	41	H,L = 2-13	-9	22	-23	-2	40	42	-8	42	-43
-5	54	-53	-2	55	-56	-8	26	-25	H,L = 2-14	-2	73	78	H,L = -8-12	H,L = -8-12	H,L = 1-12	H,L = 1-12				
-1	11	-9	H,L = -6-14	-6	17	18	H,L = -9-13	-2	11	-11	-3	31	-31	-2	48	49	-2	149	-160	
-7	17	17	-2	35	35	-4	93	-93	H,L = -7-13	-1	13	13	-5	36	-37	0	50	51		
-5	13	12	H,L = -5-14	-2	35	35	0	38	-39	H,L = -7-13	-3	26	21	H,L = -7-12	-4	50	50			
-3	27	-26	-4	29	28	H,L = 3-14	-3	24	-24	-1	5	-6	-4	44	-46	-2	46	47		
H,L = 2-15	-7	28	-2	7	-5	-4	45	45	H,L = -6-13	-5	14	15	-9	41	41	H,L = 3-15				
-1	22	22	-2	6	8	-2	76	-77	H,L = -6-13	-5	14	15	-9	41	41	H,L = 3-15				
H,L = 3-15	-5	33	33	H,L = -4-14	0	8	8	-1	9	9	-1	11	12	-2	24	24	0	130	-133	
-3	17	17	-4	31	-32	H,L = 4-14	H,L = -5-13	H,L = 4-14	H,L = -5-13	H,L = 4-15	-4	51	-53	H,L = 2-12	H,L = 2-12	H,L = 2-12				
-1	22	22	-2	6	8	-8	16	-17	-3	17	17	-9	13	14	-4	51	-53			
H,L = 3-15	0	18	-18	H,L = -3-14	-6	64	65	-1	14	-14	-7	11	11	H,L = -5-12	H,L = -5-12	H,L = -5-12				
-7	17	-17	H,L = -3-14	-2	48	49	H,L = -4-13	-5	14	-14	-6	60	61	H,L = 3-12	H,L = 3-12	H,L = 3-12				
-3	44	43	-6	34	-36	0	36	-37	-5	15	15	-3	29	-29	-8	47	-48			
H,L = 4-15	-2	38	-38	H,L = 5-14	-7	13	-12	-1	12	12	-1	12	12	-6	29	-30	0	120	-119	

-9	29	-29	-1	19	18	-4	57	57	-8	26	26	-1	25	25	-5	41	
-7	33	-34	H,L=	7	-9	-?	76	75	-10	67	79	-6	21	21	H,L=	-6	
-5	17	-18	-9	11	-10	0	62	60	-8	24	-26	-4	111-109	-/	13	-7	
-1	34	35	-7	39	39	H,L=	-5	-8	-8	10	-10	-2	46	-46	-5	41	
H,L=	0	-9	-1	16	-16	H,L=	31	-31	-4	183-200	0	126-129	-3	10	-9	H,L=	2
-3	20	21	-5	26	26	0	82	79	-8	100	106	-4	88	91	-5	36	
-1	54	-56	-1	15	-14	H,L=	8	-9	-6	8	8	-2	85	-89	-1	37	
H,L=	1	-9	H,L=	9	-9	-5	16	16	H,L=	-4	-8	-8	57	56	H,L=	-5	
-9	23	25	-5	16	16	-6	60	-60	-6	28	-29	H,L=	2	-8	-7	47	
H,L=	2	-9	H,L=	9	-9	-1	20	21	-8	17	15	-4	16	17	-/	-5	
-7	19	-20	-1	20	21	-4	68	-65	0	65	-57	-6	9	10	H,L=	3	
-5	28	30	H,L=	10	-9	-2	86	-85	H,L=	3	-8	-6	73	74	-/	40	
-3	25	-26	-5	18	-19	0	141	141	-8	5	4	-4	17	17	-3	35	
-1	17	19	-3	29	32	H,L=	-3	-8	-6	65	69	-2	118	126	-5	55	
H,L=	2	-9	-1	34	-37	-8	28	28	-4	57	50	0	33	-35	H,L=	1	
-7	34	35	H,L=	11	-9	-6	55	54	-2	40	-39	H,L=	10	-8	-9	45	
-3	38	41	-5	19	21	-4	125-125	0	117-117	-6	86	-88	-1	38	-1	37	
-5	50	53	-3	11	13	-2	25	-24	H,L=	4	-8	-4	42	44	-1	40	
H,L=	3	-9	-3	34	-39	0	156-155	-10	28	-30	-2	25	26	-1	25	-7	
-7	6	-4	H,L=	12	-9	-8	35	-37	0	75	86	H,L=	-2	-7	-3	51	
-1	27	-28	-5	19	21	-4	72	70	H,L=	11	-8	-7	47	-47	-1	48	
-3	9	-10	H,L=	-10	-8	-6	19	19	-2	89	89	-6	20	-21	-5	52	
H,L=	4	-9	-2	14	15	-4	134	135	0	7	5	-4	73	-82	-1	53	
-9	49	-50	0	116	122	-2	125-128	H,L=	5	-8	-2	24	27	-1	26	-9	
-7	12	-13	H,L=	-9	-8	0	18	-19	-8	33	-31	0	8	9	H,L=	4	
-5	5	5	-4	90	-94	H,L=	-1	-8	-6	47	-47	H,L=	12	-8	-1	51	
-3	8	6	-2	35	-35	-10	9	12	-4	7	-7	-4	14	-15	-5	52	
-1	7	5	0	16	17	-8	81	-82	-2	144	143	-2	46	-53	-3	53	
H,L=	5	-9	H,L=	-8	-8	-6	84	86	0	115	115	H,L=	-10	-7	-1	53	
-7	33	-32	-4	17	-17	-4	24	24	H,L=	6	-8	-1	8	-10	H,L=	0	
H,L=	6	-9	-2	92	-92	-10	207	220	H,L=	-9	-7	-9	38	38	H,L=	6	
-3	41	42	0	68	-69	-8	57	-60	-3	13	-15	-7	18	-18	-5	31	
-1	43	-43	H,L=	-7	-8	-6	71	-70	-1	16	17	-5	51	-53	H,L=	6	
H,L=	6	-9	-6	52	52	-10	39	-40	-4	66	-63	H,L=	-8	-7	-3	43	
-9	42	42	-4	43	43	-6	144-150	-2	33	-32	-3	23	24	-1	36	-1	
-7	14	-15	-2	18	17	-4	37	40	0	130	129	-1	14	-14	H,L=	1	
-5	20	19	0	62	-61	-2	34	35	H,L=	7	-8	-9	42	44	-9	22	
-3	24	-24	0	234	259	-10	33	33	H,L=	-6	-8	-5	13	12	-7	50	

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC									
-3	16	14	H,L = -6	-6	-6	35	35	-6	18	16	-5	51	-52	-9	7	-7	7	-4	-5	32	-30	-5	32	-30								
-1	16	-16	-8	6	-4	-4	21	-21	-4	70	-67	H,L = -9	-5	-1	36	36	-5	32	-30	-1	18	-17	H,L = 8	-5								
H,L = 8	-7	-6	84	84	-2	34	69	-2	9	7	H,L = -8	-5	-1	26	27	-5	52	53	-1	18	-17	H,L = 8	-5									
-9	22	-22	-4	20	-19	0	31	-63	0	14	-14	H,L = 7	-6	-1	5	-7	-1	52	-55	-9	17	17	H,L = 8	-5								
-7	27	-28	-2	29	28	-10	H,L = 1	-6	H,L = 7	-6	H,L = -7	-5	H,L = 7	-5	H,L = 1	-5	H,L = 1	-5	-1	27	-26	-3	7	-1								
-5	30	30	0	49	-47	-10	35	-35	-8	25	25	H,L = -6	-5	-2	54	-53	-5	59	63	H,L = 9	-5	-5	15	-14	H,L = 9	-5						
-3	30	31	H,L = -5	-6	-6	6	63	61	0	21	20	-6	47	-47	-3	50	-50	-9	35	-36	-5	15	-14	H,L = 9	-5							
H,L = 9	-7	-3	5	5	-4	43	46	-4	19	-11	-4	19	-11	-1	8	8	-1	25	-26	-3	7	-1	H,L = 9	-5								
-9	25	-24	-6	12	-12	-10	39	-32	-2	54	-53	H,L = -6	-5	H,L = -6	-5	H,L = 1	-5	H,L = 1	-5	-1	27	-26	-3	7	-1	H,L = 9	-5					
-7	49	-49	-4	63	61	-8	21	20	-8	23	-25	H,L = 2	-6	-10	43	48	-3	15	15	-7	58	58	-13	15	16	-9	26	26				
-5	19	-18	-2	50	-48	-19	16	48	-10	43	48	H,L = 2	-6	-10	43	48	-3	15	15	-5	21	21	-5	10	-1	H,L = 9	-5					
-3	23	23	H,L = 51	49	-2	51	49	-19	16	48	H,L = 2	-6	-10	43	48	-3	15	15	-5	21	21	-5	10	-1	H,L = 9	-5						
-1	25	20	H,L = -4	-6	-8	23	22	-8	23	22	H,L = 2	-6	-10	43	48	-3	15	15	-5	21	21	-5	10	-1	H,L = 9	-5						
H,L = 10	-7	-8	72	-73	-6	30	31	-6	36	35	H,L = -5	-5	-5	28	28	-5	28	28	-1	13	-14	H,L = 10	-5	H,L = 10	-5							
-7	18	-18	-4	55	-54	-4	13	6	-4	33	-32	H,L = 124	-124	-4	33	-32	-5	28	28	-1	13	-14	H,L = 10	-5	H,L = 10	-5						
-5	47	-48	-2	25	23	-2	7	-3	-2	25	-25	H,L = 23	-23	-2	19	19	-3	19	19	-5	94	-102	-7	32	32	H,L = 10	-5					
-1	11	-11	0	52	-49	0	160	-99	H,L = 9	-6	H,L = 9	-6	H,L = 9	-6	H,L = 9	-6	H,L = 9	-6	-1	16	-15	-11	25	26	-3	12	-13	H,L = 10	-5			
H,L = 11	-7	0	52	-49	-8	70	73	-8	70	73	H,L = 3	-6	-8	40	40	-8	40	40	-1	18	-18	H,L = 4	-5	H,L = 4	-5	-1	18	18	H,L = 10	-5		
-7	18	18	-6	45	-44	-6	27	-29	-6	44	44	H,L = 45	-44	-6	44	44	-9	35	-34	H,L = 3	-5	H,L = 3	-5	-1	18	18	H,L = 10	-5				
-5	13	14	-4	68	68	-4	68	68	H,L = 4	-6	H,L = 4	-6	H,L = 4	-6	H,L = 4	-6	H,L = 4	-6	-5	8	7	-5	8	7	H,L = 10	-5						
-3	32	-35	-4	14	13	-4	68	68	H,L = 10	-6	H,L = 10	-6	H,L = 10	-6	H,L = 10	-6	H,L = 10	-6	-3	33	-33	-5	23	-23	-3	15	16	H,L = 10	-5			
-1	8	9	-2	42	-41	-2	200	-200	H,L = 42	-41	H,L = 42	-41	H,L = 42	-41	H,L = 42	-41	H,L = 42	-41	-1	24	22	-3	91	-90	-1	11	11	H,L = 11	-5			
H,L = 12	-7	0	47	45	0	31	30	-6	11	10	H,L = 11	-6	H,L = 11	-6	H,L = 11	-6	H,L = 11	-6	-7	36	-36	-9	57	61	H,L = 12	-5						
-5	15	15	H,L = -2	-6	H,L = 4	-6	-8	19	-17	H,L = -3	-5	H,L = -3	-5	H,L = -3	-5	H,L = -3	-5	H,L = -3	-5	-7	17	17	-7	7	7	H,L = 11	-5					
-3	23	24	-10	54	54	-10	24	25	-4	17	17	H,L = 54	-54	-4	17	17	-4	17	17	-7	7	5	H,L = 4	-5	H,L = 4	-5	-5	20	-22	H,L = 10	-5	
H,L = -10	-6	-8	23	24	-8	26	-24	-2	54	55	H,L = 54	-54	-6	56	-57	-6	56	-57	-7	7	5	H,L = -2	-5	H,L = -2	-5	-3	13	12	H,L = 11	-4		
-2	12	12	-6	56	55	-6	118	117	H,L = 11	-6	H,L = 11	-6	H,L = 11	-6	H,L = 11	-6	H,L = 11	-6	-3	25	24	-5	8	9	-2	19	-19	H,L = 10	-5			
0	32	-32	-4	18	-17	-4	55	-55	H,L = -4	-17	H,L = -4	-17	H,L = -4	-17	H,L = -4	-17	H,L = -4	-17	-7	7	5	H,L = 4	-5	H,L = 4	-5	0	71	-73	H,L = 10	-4		
H,L = -9	-6	-2	28	-27	-2	127	124	-2	15	-15	H,L = 28	-27	-2	15	-15	-9	44	44	-1	35	-32	-7	58	57	H,L = -11	-4	H,L = -11	-4	H,L = 12	-5	H,L = 12	-5
-4	27	27	0	47	-46	0	76	78	-5	18	-18	H,L = 47	-46	-5	18	-18	-11	25	-26	-5	8	9	-4	59	61	H,L = 12	-5					
-2	14	-13	H,L = -1	-6	H,L = 5	-6	H,L = 12	-6	-3	18	-19	H,L = 12	-6	-3	18	-19	-3	25	24	-5	8	9	-2	50	-52	H,L = 12	-5					
0	31	31	-10	32	-31	-10	89	-89	-4	75	-77	H,L = 32	-31	-4	75	-77	-1	32	28	-5	41	40	-2	86	88	H,L = 12	-5					
H,L = -8	-6	-8	26	25	-8	44	43	-2	7	-8	H,L = -8	-6	-2	7	-8	-9	15	15	-1	33	32	-4	85	-86	H,L = -9	-4						
-4	41	-42	-6	33	32	-6	50	-48	0	19	-21	H,L = -10	-5	-7	42	41	H,L = 6	-5	H,L = 6	-5	-6	73	-75	H,L = -8	-4	H,L = -8	-4	H,L = -8	-4			
-2	26	26	-4	24	24	-4	66	63	H,L = -10	-5	H,L = -10	-5	H,L = -10	-5	H,L = -10	-5	H,L = -10	-5	-7	42	41	-7	42	41	-7	42	41	H,L = -8	-4			
H,L = -8	-6	-2	111	-111	-2	24	-23	-3	25	27	H,L = -8	-6	-3	25	27	-5	25	27	-5	25	27	-5	25	27	H,L = -8	-4						
H,L = -7	-6	0	6	-5	0	114	112	-1	25	-25	H,L = -7	-6	-1	25	-25	-3	57	-57	-3	10	-11	-2	34	34	H,L = -8	-4						
-4	22	23	H,L = 0	-6	H,L = 6	-6	H,L = -9	-5	-1	31	-29	H,L = -9	-5	-1	31	-29	-1	29	28	0	92	91	H,L = -7	-4	H,L = -7	-4	H,L = -7	-4				
-2	74	-74	-8	38	-38	-10	14	13	-5	16	18	H,L = -8	-5	-5	16	18	-9	12	-11	-11	33	-33	-9	12	-11	H,L = -8	-5					
0	36	35	-10	44	-43	-8	70	-68	H,L = -8	-5	H,L = 0	-5	H,L = 7	-5	H,L = 7	-5	H,L = 7	-5	-6	16	-16	-6	16	-16	H,L = -8	-5						

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	
..	0	66	-62	H,L=	5	-2	H,L=	12	-2	-9	19	19	-11	17	-17	-3	24	24	H,L=	-5	0	H,L=	-5	0
H,L=	-1	-2	-10	36	34	-6	28	28	-7	31	30	-9	26	-25	-1	6	-3	-8	53	-51	H,L=	10	-1	
-10	22	-22	-8	52	49	-4	11	12	-5	65	64	-7	38	-36	-1	-6	55	-54	-4	62	-61	H,L=	10	-1
-8	6	7	-4	56	55	-2	44	45	-3	56	54	-5	80	78	-9	23	23	-6	55	-54	-7	20	-22	
-6	139-137	-2	108-104	0	34	-35	-1	43	-41	-3	63	-58	-7	20	-22	-2	21	18	-6	150-142	0	H,L=	0	
-4	11	.11	0	75	70	H,L=-11	-1	H,L=-2	-1	-1	51	49	-5	9	-8	0	147	141	H,L=	-4	0	H,L=	-4	0
-2	8	-8	H,L=	6	-2	-3	20	21	-9	36	-35	-11	34	33	-1	23	-24	-8	29	29	H,L=	11	-1	
0	31	28	-10	55	53	H,L=-10	-1	-7	36	-35	-9	49	-47	H,L=	11	-	-6	21	-20	-4	111-114	H,L=	11	-1
-6	9	-8	-8	21	-20	-3	38	-39	-5	48	47	-9	49	-47	-1	51	49	-2	75	-74	-1	14	-14	
-4	59	-60	-2	54	53	-3	13	-15	-3	19	20	-5	29	-28	-5	10	11	0	133	125	-1	9	9	
-2	14	14	0	143-144	H,L=	-3	-1	H,L=	-3	-11	19	18	H,L=	5	-1	H,L=	12	-1	H,L=	-3	0	H,L=	-3	0
0	31	-35	H,L=	7	-2	-7	15	13	-9	49	-46	-9	37	36	-3	23	23	-10	12	13	H,L=	11	0	
H,L=	1	-2	-10	62	-60	-5	27	27	-7	48	-46	-7	57	-55	-1	13	-14	-8	65	64	H,L=	-11	0	
-10	16	16	-8	42	40	-3	34	35	-5	72	-70	-5	36	-35	H,L=	-11	0	-6	67	65	-3	9	9	
-8	64	63	-6	40	-38	-1	29	-30	-3	24	-19	-3	9	-7	-2	86	90	-4	75	-72	H,L=	-10	0	
-6	37	38	-4	101	98	H,L=	-7	-1	-1	6	6	-1	9	9	H,L=	-10	0	-2	104-100	-	H,L=	-10	0	
-4	51	57	-2	14	12	-7	37	-38	H,L=	0	-1	H,L=	6	-1	-4	9	12	0	124-126	-	H,L=	-2	0	
-2	31	26	0	45	43	-5	35	37	-11	28	27	-11	19	17	-2	28	-29	H,L=	-1	0	H,L=	-1	0	
0	35	35	H,L=	8	-2	-3	7	7	-9	42	41	-9	26	25	0	136	140	-10	31	-30	H,L=	-9	0	
H,L=	2	-2	-8	71	-69	-1	34	33	-7	15	-15	-7	20	19	H,L=	-9	0	-8	33	31	-5	53	-51	
-10	25	-26	-6	11	11	H,L=	-6	-1	-5	32	-31	-5	25	-24	-6	18	19	-6	47	46	-7	16	-16	
-8	20	-22	-4	27	-25	-7	16	-16	-3	5	-5	-3	53	-51	-4	113-116	-4	109	104	-7	11	-11		
-6	21	23	-2	87	86	-5	49	-48	-1	7	-9	-1	13	-11	-2	29	-29	-2	142-134	-	H,L=	-10	0	
-4	13	13	0	6	7	-3	36	35	H,L=	1	-1	H,L=	7	-1	0	32	-32	0	124-119	-	H,L=	-1	0	
-2	76	73	H,L=	9	-2	-1	14	-14	-11	13	13	-11	18	-17	H,L=	-8	0	H,L=	-1	0	H,L=	-1	0	
0	74	-71	-6	70	-68	H,L=	-5	-1	-9	45	42	-7	40	38	-4	17	18	-10	12	-11	H,L=	0	0	
H,L=	3	-2	-4	7	8	-9	31	33	-7	39	37	-5	33	35	-2	127	-128	-8	64	-62	H,L=	0	0	
-10	45	-45	-2	52	-51	-7	28	-28	-5	20	-3	27	26	0	49	-47	-6	40	38	H,L=	-1	0		
-8	35	-36	H,L=	10	-12	-5	25	-24	-3	22	18	-1	42	-41	H,L=	-7	0	-4	29	28	H,L=	0	0	
-6	77	-75	-8	15	-14	-3	64	-63	-1	37	36	H,L=	8	-1	-6	97	97	-2	303	317	H,L=	0	0	
-4	25	25	-6	14	15	-1	39	38	H,L=	2	-1	-9	23	-22	-4	29	29	-8	17	17	H,L=	-6	0	
-2	42	35	-4	23	-23	H,L=	-4	-1	-11	28	-28	-7	25	-23	-2	59	59	H,L=	0	0	H,L=	0	0	
0	17	8	-2	7	-9	-9	10	9	-9	9	-8	-5	55	54	0	76	-73	-10	19	-19	H,L=	9	-1	
H,L=	4	-2	0	53	-53	-7	49	48	-7	26	26	-1	45	45	H,L=	-6	0	-8	17	17	H,L=	-6	0	
-10	36	34	H,L=	11	-12	-5	22	-22	-5	10	-6	H,L=	9	-1	-6	27	-27	-6	150-142	-	H,L=	0	0	
-4	43	-42	-8	36	-36	-3	12	-11	-3	22	24	-9	27	-27	-4	70	70	-4	50	48	H,L=	0	0	
-2	127	120	-4	35	35	-1	32	-30	-7	4	-5	-7	4	-5	-2	77	75	-2	7	6	H,L=	-3	-1	
0	28	-29	-4	6	-4	-5	41	-40	0	82	80	H,L=	3	-1	0	82	80	H,L=	1	0	H,L=	1	0	

K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC			
-10	67	64	-10	33	34	-4	123	-119	-1	26	-29	-7	25	24	-9	82	79	-1	14	-13	-1	14	-13			
-8	30	-28	H,L=	2	6	-2	16	-14	H,L=-10	1	-5	93	-90	H,L=	6	1	H,L=-12	2	H,L=-12	2	H,L=-11	2				
-6	49	48	-4	10	-11	0	83	80	-3	13	-14	-3	27	25	-5	45	43	0	33	-35	0	33	-35			
-4	311	-340	H,L=	-3	6	H,L=	10	0	-1	6	8	-1	71	-69	H,L=	5	1	H,L=-11	2	H,L=-11	2	H,L=-10	2			
-2	5	5	-10	57	-57	0	136	140	H,L=-9	1	H,L=	0	1	-5	33	-33	-2	37	-40	H,L=-10	2	H,L=-10	2			
0	66	-63	H,L=	-4	6	H,L=	7	0	-3	11	11	-9	64	63	-3	42	-40	0	53	-53	H,L=-9	2	H,L=-9	2		
H,L=	2	6	0	48	-46	-10	23	22	H,L=-8	1	-7	13	-12	-1	29	-27	-6	31	-31	-6	31	-31				
-10	45	-43	H,L=	10	5	-8	62	60	-5	12	13	-5	37	34	H,L=	6	1	-4	12	11	0	53	-53			
-8	131	131	-7	22	-22	-6	7	6	-3	26	25	-3	5	-8	-7	55	52	H,L=-9	2	H,L=-9	2					
-6	46	-44	H,L=	4	-18	-4	82	-80	-1	18	-19	-1	6	6	H,L=	7	1	-6	31	-31	-6	31	-31			
-4	34	33	-2	16	15	-2	66	-83	-5	19	19	-9	15	15	-3	56	55	H,L=	8	2	H,L=	8	2			
-2	307	-319	H,L=	1	-18	0	77	-73	-7	22	-23	-11	23	23	-1	31	-31	-6	9	-9	-6	9	-9			
H,L=	-5	20	-6	8	-7	H,L=	5	0	-5	19	19	-7	53	51	H,L=	8	1	-4	24	-25	0	30	31			
0	67	-65	H,L=	2	6	-10	14	-13	-3	12	-10	-7	53	51	H,L=	8	1	-4	27	26	-4	30	31			
H,L=	-5	19	0	125	-119	-8	41	40	-1	47	47	-5	6	2	H,L=	8	1	-4	24	-25	H,L=	8	1			
-1	27	26	H,L=	3	0	-6	60	58	H,L=-6	1	-3	7	-7	-9	14	-14	-9	14	-14	-2	51	52				
H,L=	4	13	-10	35	34	-4	74	74	-5	72	-72	-1	14	-14	-7	46	-45	0	7	1	H,L=-7	2				
-3	5	5	-8	32	-30	-2	64	-63	-1	19	-19	H,L=	2	1	-5	25	24	-9	17	-16	-2	88	-88			
H,L=	0	13	-6	138	131	0	48	-47	H,L=-5	1	-11	38	-37	-3	10	9	-9	42	44	-1	47	47	0	45	43	
H,L=	-7	26	-4	22	22	H,L=	9	0	-9	42	44	-9	11	-8	-1	46	-45	H,L=	9	1	H,L=	9	1			
H,L=	-3	11	-2	130	121	-8	51	-49	-3	57	-56	-7	19	20	H,L=	9	1	H,L=	-6	2	H,L=	-7	2			
-9	38	39	0	125	-126	-6	43	41	-1	23	-21	-5	43	42	-9	17	-16	-8	15	-15	-2	88	-88			
H,L=	8	10	-4	43	42	H,L=	-4	1	H,L=-4	1	-3	11	-6	-7	15	-15	-6	76	77	H,L=	10	1	H,L=-5	2		
0	54	-55	-10	59	-57	-2	136	135	-9	9	8	-1	29	-27	-5	58	-59	-4	21	-20	-2	17	-16			
H,L=	4	10	-8	15	15	0	33	-32	-7	56	54	H,L=	3	1	-3	18	18	-2	15	-16	-2	17	-16			
-8	8	9	-6	37	-36	H,L=	10	0	-5	57	55	-11	26	-28	-1	14	-13	0	147	-144	H,L=	10	1	H,L=-5	2	
H,L=	11	8	-4	116	110	-8	10	-9	-3	34	33	-9	56	-54	H,L=	10	1	H,L=	10	1	H,L=	10	1			
-4	88	-91	-2	107	102	-6	106	-105	-1	7	-6	-7	47	-45	-9	34	34	-6	17	-16	-2	50	-49			
H,L=	2	8	0	133	125	-4	17	17	H,L=-3	1	-5	24	21	-7	25	-26	-4	110	108	-2	110	108				
H,L=	0	18	-19	H,L=	5	0	-2	29	29	-9	21	-20	-3	24	23	-5	17	-17	-2	50	-49	0	75	70		
H,L=	-6	8	-10	-8	28	26	H,L=	11	0	-7	11	-11	-1	49	46	-3	33	-33	0	75	70	H,L=	-4	2	H,L=-4	2
H,L=	11	12	-8	56	-54	-4	121	-123	-5	25	25	H,L=	4	1	-1	12	-12	H,L=	11	1	H,L=	11	1	H,L=	11	1
H,L=	-1	7	-9	42	-40	-2	24	25	-3	80	77	-11	31	31	H,L=	11	1	-8	77	-76	-6	32	31			
-5	28	-23	-4	55	-51	H,L=	12	0	-1	17	-17	-9	13	-13	-7	32	33	-6	32	31	-4	66	-63			
H,L=	-3	7	-2	68	86	-6	16	-16	H,L=	-2	1	-7	40	-39	-5	13	14	-4	66	-63	-2	37	-40			
H,L=	10	-10	0	148	141	-4	15	16	-9	23	-22	-5	87	-85	-3	19	-19	-2	114	112	H,L=-10	2				
H,L=	-5	51	51	H,L=	6	0	-2	81	-85	-1	94	90	-3	43	39	-1	17	16	0	28	-29	H,L=-10	2			
H,L=	-6	7	-10	-10	16	14	H,L=-12	1	H,L=-1	1	-1	15	15	H,L=	12	1	H,L=	12	1	H,L=-3	2	H,L=-3	2			
-7	31	-31	-8	23	22	-1	22	26	-11	23	23	-1	15	15	-5	13	14	-8	52	51	-6	72	-71			
H,L=	-11	1	-9	11	-11	-11	H,L=	5	1	-11	34	32	-3	28	29	-5	13	14	-6	72	-71	-5	28	29		

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC		
-4	38	36	-4	64	-65	-4	40	-39	-5	6	-5	-9	33	33	-4	95	-95	-5	6	-5	-9	15	-15		
-2	134	-128	-2	3	2	-2	6	7	-3	12	15	-3	12	15	-2	25	25	-5	14	-15	-7	25	-24		
0	15	8	0	66	-62	0	15	-15	-7	25	-24	-1	67	68	-3	16	-15	-5	74	73	H,L = 2	3			
H,L = -2	2	H,L = 3	H,L = 2	H,L = 9	H,L = 2	H,L = 9	H,L = 2	H,L = 9	H,L = 2	H,L = 9	H,L = 2	H,L = 9	H,L = 2	H,L = 9	H,L = 2	H,L = 9	H,L = 2	H,L = 9	H,L = 2	H,L = 9	H,L = 2	H,L = 9	H,L = 2		
-10	64	62	-10	29	30	-8	44	43	-3	21	20	-7	32	-34	-7	28	2/	-6	38	-38	-5	83	-87		
-8	10	-11	-8	59	59	-6	3	7	-1	19	18	-5	83	-87	-5	7	-5	-2	141	-138	-1	19	18		
-2	55	-48	-2	211	-201	0	3	-9	-7	38	-37	H,L = 3	H,L = 3	H,L = 3	H,L = 10	H,L = 10	H,L = 10	H,L = 10	H,L = 10	H,L = 10	H,L = 10	H,L = 10	H,L = 10		
0	74	-71	0	111	163	H,L = 10	2	H,L = -4	-3	-5	19	-18	-11	11	11	-7	13	12	-6	74	74	-1	19	18	
H,L = -1	2	H,L = 4	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2	H,L = 2		
-10	43	-47	-6	148	146	-6	14	14	-1	34	31	-5	5	-3	H,L = 11	H,L = 11	H,L = 11	H,L = 11	H,L = 11	H,L = 11	H,L = 11	H,L = 11	H,L = 11		
-8	41	40	-4	43	-42	-2	19	19	H,L = -3	3	-3	54	-54	-1	7	6	-7	76	75	H,L = 12	3	H,L = -4	4		
0	35	35	-10	96	-92	0	48	50	H,L = -2	3	-5	17	17	-7	76	75	-7	76	75	H,L = 12	3	H,L = -3	4		
H,L = 0	2	-8	17	16	H,L = 12	2	H,L = -2	3	-5	17	17	-5	17	17	-7	76	75	-7	76	75	H,L = 12	3	H,L = -4	4	
-10	39	-38	-6	44	-42	-4	38	-38	H,L = -2	3	-5	17	17	-7	76	75	-7	76	75	H,L = 12	3	H,L = -3	4		
-2	25	-18	-10	96	-92	-2	23	-24	H,L = -2	3	-5	17	17	-7	76	75	-7	76	75	H,L = 12	3	H,L = -4	4		
-8	37	-36	-4	115	110	-1	11	-11	H,L = -1	3	-7	11	11	-1	11	11	-5	9	10	-8	20	21	H,L = -12	4	
-6	66	65	-2	82	-79	0	10	-9	H,L = -1	3	-5	16	-16	H,L = 4	H,L = 4	H,L = 4	-5	16	17	-4	161	160	H,L = 4	5	
-4	8	9	0	117	114	H,L = -11	3	-3	76	-74	-11	45	-44	-11	45	-44	-5	30	-32	-10	13	14	H,L = -3	4	
-10	39	-38	-3	22	24	-2	23	-24	H,L = -1	3	-7	17	-17	H,L = -1	H,L = -1	H,L = -1	-7	76	75	-7	76	75	H,L = -3	4	
-2	25	-18	-1	11	-11	H,L = -10	3	-1	31	-31	-5	65	62	H,L = 6	H,L = 6	H,L = 6	-6	26	-25	H,L = -12	4	H,L = -3	4		
0	31	-35	-10	14	14	H,L = -10	3	-3	76	-74	-11	45	-44	-11	45	-44	-5	30	-32	-10	13	14	H,L = -3	4	
H,L = 1	2	-8	96	-94	H,L = -8	3	-3	22	-1	22	-9	12	-11	H,L = -11	H,L = -11	H,L = -11	-7	76	75	-7	76	75	H,L = -3	4	
-10	41	-40	-6	22	21	-3	15	16	H,L = -9	3	-7	17	-17	H,L = -12	H,L = -12	H,L = -12	-7	76	75	-7	76	75	H,L = -3	4	
H,L = -2	1	-4	118	-115	H,L = -9	3	-7	56	H,L = -9	3	-7	17	-17	H,L = -12	H,L = -12	H,L = -12	-7	76	75	-7	76	75	H,L = -3	4	
-7	66	-64	-2	62	59	-1	23	23	-5	14	14	H,L = 6	H,L = 6	H,L = 6	-5	62	62	-6	188	186	H,L = -3	4			
-5	18	-19	0	73	-71	H,L = -8	3	-3	45	42	-11	9	9	H,L = -10	H,L = -10	H,L = -10	0	89	88	-6	117	114	H,L = -3	4	
-3	90	-85	H,L = 7	2	-5	29	-30	-1	83	-82	-9	59	-58	H,L = -9	H,L = -9	H,L = -9	-4	62	-60	-4	62	-60	H,L = -2	4	
H,L = 1	2	-8	66	65	H,L = -7	3	-11	24	-24	-5	23	-22	-4	31	31	H,L = -9	H,L = -9	H,L = -9	0	142	143	H,L = -1	4		
-6	11	-11	-6	65	-63	-7	9	9	-5	86	87	-3	10	9	-2	121	123	-10	48	44	H,L = -2	4			
-4	39	43	-4	40	39	-3	59	-58	-3	41	41	-1	4	3	-6	26	26	-8	21	-19	H,L = -4	4			
-2	15	-16	-2	98	-97	-1	29	29	-7	18	-17	H,L = 7	H,L = 7	H,L = 7	-6	26	26	-2	113	-109	H,L = -4	4			
0	32	28	0	64	62	H,L = -6	3	-1	15	16	-9	17	15	H,L = -8	H,L = -8	H,L = -8	-6	74	-76	-6	43	41	H,L = -1	4	
H,L = 2	2	H,L = 8	2	-7	60	61	H,L = 1	3	-7	21	-21	-4	50	50	-4	125	-126	-10	12	10	H,L = -4	4			
-10	34	35	-10	66	65	-5	7	-7	-11	22	-5	22	-20	-2	31	29	-2	55	-58	-2	196	-213	H,L = -4	4	
-8	20	-22	-8	5	-5	-3	30	29	-9	40	-41	-3	17	17	-3	17	17	0	133	131	0	196	-213	H,L = -7	4
-6	32	-35	-1	58	-56	-7	22	-21	H,L = 8	3	-7	22	-21	H,L = -7	H,L = -7	H,L = -7	0	196	-213	H,L = 0	-4	H,L = 0	-4		

K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC
-10	19	-18	-6	22	22	-3	16	-15	-9	23	-22	-7	21	-21	-2	13	13	0	208	225	H,L =	0	
-8	73	73	-4	158	155	H,L =	-8	5	-7	47	-48	-5	36	-35	H,L =	-7	6	H,L =	0	6	H,L =	0	
-6	43	42	-2	51	49	-3	23	-23	-5	57	60	-3	27	26	-6	19	-18	-10	93	94	H,L =	6	
-4	145	152	0	16	-16	H,L =	-7	5	-3	21	23	-4	10	9	-6	26	28	-6	26	28	H,L =	6	
-2	80	-93	H,L =	7	4	-7	28	29	-1	96	104	-9	25	25	-2	18	17	-4	119	-128	H,L =	6	
0	126	-140	-8	69	-68	-5	18	19	H,L =	1	5	-7	34	-32	0	21	20	-2	26	28	H,L =	6	
H,L =	1	4	-6	8	-9	-3	11	11	-11	17	16	-5	35	-34	H,L =	-6	6	0	80	-83	H,L =	1	
-8	69	-71	-4	18	17	-1	5	-5	-9	41	-42	H,L =	8	5	-8	24	-23	H,L =	1	6	H,L =	1	
-6	66	69	-2	135	132	H,L =	-6	5	-7	27	-29	-9	47	47	-6	42	-42	-10	12	-15	H,L =	6	
-4	85	93	0	68	66	-5	9	10	-5	100	-109	-7	24	25	-4	42	-41	-3	70	74	H,L =	6	
-2	120	135	H,L =	5	4	-3	25	24	-3	13	-12	-5	7	3	-2	49	48	-6	15	-16	H,L =	6	
0	195	-206	-6	71	-69	H,L =	-5	5	-1	19	18	-3	46	-45	0	14	-14	-4	52	51	H,L =	6	
H,L =	2	4	-4	28	-27	-9	21	-22	H,L =	2	5	-1	16	16	H,L =	-5	6	-2	84	-90	H,L =	6	
-10	36	-38	-2	50	-49	-7	32	-31	H,L =	3	5	-8	52	51	0	5	-5	H,L =	2	6	H,L =	2	
-8	32	-35	0	93	91	-5	5	5	-9	41	45	-7	55	54	-6	39	-39	H,L =	2	6	H,L =	2	
-6	102	-110	H,L =	9	4	-3	9	-9	-7	6	-7	-5	21	22	-4	7	-6	-8	33	-35	H,L =	6	
-4	112	116	-6	25	26	-1	22	20	-5	37	-39	-3	12	12	-2	6	-4	-6	39	43	H,L =	6	
-2	76	75	-4	82	-82	H,L =	-4	5	-3	54	-54	-1	31	-30	0	114	112	-2	115	115	H,L =	6	
0	134	140	-2	31	-31	-5	22	-20	-1	32	-30	H,L =	10	5	H,L =	-4	6	0	7	2	H,L =	6	
H,L =	3	4	0	85	-86	-3	6	-5	H,L =	3	5	-5	40	41	-8	32	33	H,L =	3	6	H,L =	3	
-10	48	51	H,L =	10	4	-1	40	38	-11	16	17	-3	11	12	-6	54	54	-10	44	-48	H,L =	6	
-8	56	-57	-8	49	49	H,L =	-3	5	-9	33	34	-1	19	19	-4	67	-65	-8	9	-9	H,L =	6	
-6	17	-17	-4	61	62	-9	20	20	-7	43	45	H,L =	11	5	-2	31	30	-6	46	-48	H,L =	6	
-4	115	-114	-2	96	-96	-5	47	-47	-5	49	51	-5	31	-32	H,L =	-3	6	-4	14	13	H,L =	6	
-2	100	96	0	26	-26	-3	8	-8	H,L =	4	-3	31	32	-8	25	24	-2	32	30	H,L =	6		
0	133	125	H,L =	11	4	-1	21	-20	-11	13	-13	H,L =	12	5	-6	18	-16	0	47	45	H,L =	6	
H,L =	4	4	-6	77	79	H,L =	-2	5	-9	10	-11	-3	18	-20	-4	71	69	H,L =	4	6	H,L =	4	
-8	68	66	-4	24	25	-9	26	25	-7	28	29	H,L =	-12	6	-2	127	-126	-8	27	-27	H,L =	6	
-6	31	-29	-2	48	48	-7	13	14	-5	27	28	0	20	-21	0	30	30	-6	26	-26	H,L =	6	
-4	52	-49	0	70	-73	-5	17	14	-3	37	36	H,L =	-11	6	H,L =	-2	6	-4	25	-24	H,L =	6	
-2	179	-176	H,L =	12	4	-7	68	-67	-1	10	-9	0	76	78	-8	87	-87	-2	45	44	H,L =	6	
0	43	-40	-4	68	71	-1	7	-4	H,L =	5	5	H,L =	-10	6	-6	38	37	0	52	-49	H,L =	6	
H,L =	5	4	-2	24	25	H,L =	-1	5	-11	31	-30	-4	70	-72	-4	54	-53	H,L =	5	6	H,L =	5	
-10	17	16	H,L =	-11	5	-9	11	-12	-9	25	-27	-2	6	8	-2	197	201	-10	41	42	H,L =	6	
-6	87	84	-3	16	18	-7	48	48	-7	26	-26	H,L =	-9	6	0	99	-99	-8	27	27	H,L =	6	
-4	25	24	-5	46	47	-5	21	21	-5	21	-21	-2	43	-43	H,L =	-1	6	-6	55	-55	H,L =	6	
-2	84	-82	-3	7	-9	-3	71	71	-3	16	-16	0	7	-7	-8	41	41	-4	19	19	H,L =	6	
0	248	-246	-1	18	19	-1	46	-48	-1	34	33	H,L =	-8	6	-6	127	-128	-2	27	-25	H,L =	6	
H,L =	6	4	-5	11	25	H,L =	0	5	-9	43	-42	-4	44	45	-4	53	51	14	11	11	H,L =	6	

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC
-10	41	40	-7	40	-39	-7	66	71	-9	35	-35	-6	9	-8	0	56	-60	0	61	-61	H,L=	2	8
-8	13	11	-5	14	-15	-5	8	-7	-5	15	16	-4	91	-90	-10	16	-15	-8	18	19	H,L=	8	8
-6	37	36	-3	22	22	-3	26	-27	-1	28	27	-2	46	45	-8	68	94	-6	34	33	H,L=	9	7
-4	55	-54	-1	15	14	-1	52	-54	H,L=	2	7	-7	23	-24	H,L=	-4	8	-6	11	-11	-4	46	41
-2	46	45	H,L=	-6	7	H,L=	-2	7	-11	47	-49	-11	47	-49	-8	48	47	-4	24	26	-2	20	-20
0	49	-47	-5	46	-46	-1	17	-17	-7	10	11	-1	18	-17	-4	72	-71	H,L=	3	8	H,L=	9	8
-8	40	39	H,L=	-5	7	H,L=	-5	7	-5	66	72	H,L=	10	7	-2	141	-139	-10	19	21	-8	26	-21
-4	67	65	-7	20	19	-3	27	28	-7	17	-18	0	7	5	-6	14	-14	-6	14	-14	0	1/	1/
-2	23	-23	-5	11	11	-1	41	-41	-3	26	-25	H,L=	-3	8	-6	138	141	-4	39	38	H,L=	10	8
0	35	35	-3	58	-56	H,L=	3	7	-1	16	16	-8	20	20	-4	12	11	-2	84	85	H,L=	11	7
-8	66	-65	H,L=	-4	7	-7	35	-37	-5	8	-9	-4	18	-19	0	156	-155	-2	122	126	0	1/	1/
-6	16	16	-7	57	57	-5	36	37	-1	12	-12	-2	98	-99	H,L=	4	8	-6	49	-49	H,L=	10	8
-4	15	-15	-3	27	27	-3	16	15	H,L=	-11	8	0	118	-117	-10	60	-63	-4	10	-10	H,L=	11	9
-2	81	81	-1	53	-52	-1	64	63	-2	44	46	H,L=	-2	8	-8	17	17	-2	36	36	H,L=	10	8
0	35	-35	H,L=	-3	7	H,L=	4	7	0	8	9	-10	28	-27	-6	70	-72	0	117	122	H,L=	11	9
-6	9	6	-1	14	-13	-11	31	34	H,L=	-10	8	-8	18	19	-4	133	134	H,L=	11	9	H,L=	11	9
-6	90	-90	H,L=	-2	7	-7	12	-12	-2	24	-25	-6	43	43	-2	25	24	-1	28	-28	H,L=	10	8
-4	11	12	-9	49	-48	-5	64	-64	0	85	86	-4	65	62	0	141	141	H,L=	4	8	H,L=	10	8
-2	29	-30	-7	15	-15	-3	25	25	H,L=	-9	8	-2	37	35	H,L=	5	8	-3	20	-20	H,L=	10	8
0	32	31	-5	21	20	-1	12	-12	-4	74	-75	0	65	-67	-10	39	40	-1	22	22	H,L=	10	8
H,L=	10	6	-1	4	4	H,L=	5	7	-2	11	-14	H,L=	-1	8	-8	79	-80	H,L=	-9	9	H,L=	-9	9
-6	17	18	H,L=	-1	7	-9	35	35	0	34	-33	-10	17	-16	-6	18	-17	-3	56	56	H,L=	6	8
-4	41	-41	-9	13	-12	-7	21	-21	H,L=	-8	8	-8	14	-13	-4	118	-118	-1	23	-23	H,L=	6	8
-2	9	6	-7	46	-47	-5	15	-16	-4	30	28	-4	51	53	-2	81	80	H,L=	-8	9	H,L=	-7	9
0	32	-32	H,L=	-2	7	-3	77	-76	-2	130	-128	-2	113	121	0	82	79	-5	20	21	H,L=	-7	9
H,L=	11	6	-3	31	32	-1	20	20	0	18	-17	0	67	67	H,L=	6	8	-1	19	19	H,L=	-7	9
-6	11	11	H,L=	-1	7	-3	11	12	H,L=	6	7	H,L=	-7	8	-10	14	-14	H,L=	-7	9	H,L=	-7	9
-4	39	40	H,L=	-10	7	-1	21	21	-5	21	-21	-2	71	-52	-6	53	-52	H,L=	-6	9	H,L=	-6	9
-3	49	-51	H,L=	0	7	-3	10	9	0	130	-129	-4	16	-16	-4	67	-66	-5	15	-16	H,L=	-5	9
H,L=	-9	7	-9	42	43	-1	43	-43	H,L=	-6	8	-2	12	-12	-2	67	-65	-3	21	-21	H,L=	-5	9
-5	13	13	-5	47	-50	H,L=	7	7	-6	56	-56	0	232	259	H,L=	7	8	-1	20	-20	H,L=	-5	9
-1	34	-34	-3	63	-67	-9	20	21	-4	100	99	H,L=	1	8	-8	33	33	H,L=	-5	9	H,L=	-5	9
H,L=	-8	7	-1	20	20	-7	9	11	-2	46	45	-10	21	22	-6	54	54	-5	24	24	H,L=	-5	9
-5	57	58	H,L=	1	7	-5	57	56	0	133	129	-8	13	-14	-6	54	54	-3	19	-18	H,L=	-5	9
-3	33	33	-3	6	7	H,L=	-5	8	-4	176	-194	-4	38	-36	-1	6	7	-2	30	-31	H,L=	-4	9
H,L=	-7	7	-9	30	31	H,L=	8	7	-8	54	-55	-2	71	-68	H,L=	-4	9						

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC			
-7	33	33	-5	11	-11	-7	11	-11	H,L=-10	10	0	74	-75	-10	53	-54	-3	35	35	
-5	11	9	-3	37	38	-2	38	39	H,L=-1	10	-6	21	-22	-1	35	35	-5	17	-16	
-3	58	58	-1	34	33	0	43	-43	H,L=-4	9	-10	50	-51	-4	58	58	-1	15	-16	
-1	43	-44	H,L=	4	9	-9	6	6	H,L=-9	10	-8	59	62	-2	13	13	-3	22	22	
H,L=-3	9	-3	-3	11	-10	-7	29	-30	H,L=	9	-4	85	90	-5	54	55	-5	26	26	
-7	37	-37	-1	15	14	-1	23	-23	H,L=-8	10	-2	18	19	-2	84	-85	-1	54	55	
-5	36	36	-1	15	14	-1	23	-23	H,L=-8	10	0	45	47	-10	18	-19	-3	27	27	
-3	6	5	-3	11	-10	-2	23	24	H,L=	0	-8	78	-80	-1	48	-49	-1	52	52	
-1	15	14	-1	23	-23	-4	33	-33	H,L=	0	-8	78	-80	-3	43	42	-5	27	-28	
H,L=-2	9	-2	H,L=	5	9	-2	23	24	H,L=-8	10	-10	18	-19	-2	63	63	-1	3	11	
-9	45	-45	-2	37	38	0	16	16	H,L=-8	10	-6	60	63	-4	11	-3	-3	22	-20	
-7	26	-26	-3	58	-58	H,L=	-7	10	-4	12	-13	-2	94	-95	H,L=-3	11	H,L=	4		
-5	28	-28	-1	16	-16	-6	8	-7	0	78	-80	0	50	49	-7	36	-37			
-3	12	-11	H,L=	6	9	-2	54	-53	H,L=	1	10	H,L=	8	10	-5	36	-36			
-1	29	29	-9	9	10	H,L=	-6	10	-10	42	-43	-8	17	-17	-3	80	-80			
H,L=-1	9	-7	54	56	-6	H,L=-6	10	-10	-8	21	-22	-6	67	68	-1	29	29			
-9	19	19	-5	40	40	-2	21	-20	-6	50	-53	-4	52	-52	H,L=-2	11	-1	42	-43	
-5	37	-38	-3	22	21	0	92	-89	-4	32	34	-2	35	35	-9	23	21	H,L=	6	
-3	15	17	-1	22	-23	H,L=-5	10	-2	16	17	H,L=	9	10	-7	68	69	H,L=	1	1	
-1	34	-37	H,L=	7	9	-8	16	-15	0	23	-24	-6	16	-17	-3	11	-10	H,L=	5	
H,L=	0	9	-9	17	-16	-6	10	11	H,L=	2	10	-4	43	44	-1	13	-12	H,L=	1	
-9	42	43	-7	0	-5	-4	83	82	-10	49	52	-2	41	-41	H,L=-1	11	-7	18	-18	
-7	11	11	-5	39	39	-2	21	-20	-6	18	-19	0	36	37	-7	26	26	H,L=	5	
-5	26	27	-3	29	29	0	35	34	-4	9	-8	H,L=	10	10	-5	60	61	H,L=	1	
-3	40	-42	H,L=	8	9	H,L=-4	10	-2	20	22	-4	19	-19	-3	53	56	-3	10	10	
-1	10	11	-7	29	-30	-8	62	-62	0	53	55	-2	21	20	-1	24	-24	H,L=	6	
H,L=	1	9	-5	12	-12	-6	11	9	H,L=	3	10	0	15	-16	H,L=	0	11	H,L=	1	
-9	14	-16	-3	10	-9	-4	32	-32	-10	22	24	H,L=-10	11	-9	28	-29	-1	28	26	
-7	38	39	-1	24	24	-2	100	98	-8	38	41	-1	31	31	-7	40	-41	H,L=	6	
-3	27	29	H,L=	9	9	0	55	-55	-6	22	23	H,L=-9	11	-5	23	24	-3	49	48	
-1	69	-71	H,L=	-7	11	-10	H,L=-3	10	-4	21	-22	-3	15	16	-3	9	8	-1	10	8
H,L=	2	9	-5	38	-40	-8	25	26	-2	65	-66	H,L=-8	11	-1	34	36	H,L=	1	11	
-3	9	8	-3	13	14	-6	89	-89	0	12	13	-5	16	-14	H,L=	1	11	H,L=	3	
-7	24	-26	-1	28	-28	-4	29	27	H,L=	4	10	-3	29	-30	-9	27	-29	-5	28	-28
-5	66	71	H,L=	10	9	-2	89	-90	-10	20	-22	H,L=-7	11	-7	21	-22	-3	23	-23	
-3	9	7	-5	14	14	-6	67	66	-6	55	56	-3	35	-35	-5	39	-40	-1	16	16
-1	14	14	-3	30	-31	H,L=	-2	10	-4	6	5	-1	10	8	-3	23	24	H,L=	8	
H,L=	3	9	-1	14	14	-6	69	69	-2	26	-27	H,L=-6	11	-7	34	34	H,L=	2		
-9	36	-39	-4	67	-67	-2	26	-27	H,L=-11	10	-2	26	-27	-7	34	34	-9	25	27	
-7	11	-12	H,L=	-11	10	-2	37	38	H,L=-8	10	-5	18	17	-7	26	-27	-5	20	-21	

K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC	K	F0	FC
-1	16	-17	-8	62	-62	0	29	-29	-1	26	26	-3	5	5	-4	19	-18	H,L =	4	14			
H,L =	9	11	-6	25	-25	H,L =	5	12	-1	32	32	-2	25	-23	-8	35	-36						
-5	21	22	-2	115	116	-6	59	59	-5	43	-43	H,L =	6	13	0	36	-37	-6	29	-36			
-3	12	12	0	68	69	-2	9	-9	-3	29	-29	-7	9	-10	H,L =	-3	14	-4	40	-41			
-1	19	-21	H,L =	-2	12	0	116	-116	-1	4	-4	-5	36	-36	-4	37	38	-2	32	32			
H,L =	10	11	-6	70	-71	H,L =	6	12	H,L =	-3	13	-3	20	20	-2	37	-38	0	19	-18			
-5	26	26	-4	44	-44	-8	12	13	-7	18	17	-1	16	9	0	7	8	H,L =	5	14			
-3	15	15	-2	41	-42	-6	14	14	-3	33	-33	H,L =	7	13	H,L =	-2	14	-3	46	47			
-1	18	18	0	114	118	-8	55	-55	H,L =	-2	13	-7	10	-11	-5	21	-20	-6	20	20			
H,L =	-11	12	H,L =	-1	12	-2	44	44	-5	24	25	-5	21	-20	-6	20	20	-2	11	-10			
0	54	-56	-9	14	14	-6	33	34	-3	11	10	-3	31	-31	-4	15	-14	0	48	48			
H,L =	-10	12	H,L =	-1	12	H,L =	7	12	H,L =	-2	13	-1	9	7	-2	81	83	H,L =	6	14			
-2	10	-9	-4	78	-79	-6	16	-17	H,L =	-3	13	H,L =	8	13	0	31	-34	-6	40	40			
C	32	-33	-2	74	-76	-4	18	18	-5	12	12	H,L =	-1	14	H,L =	-1	14	-4	26	-26			
H,L =	-9	12	0	130	-133	-2	76	78	-3	32	33	-3	18	-18	-8	20	19	-2	12	10			
H,L =	-10	12	H,L =	0	12	0	59	60	-1	11	-12	-1	11	-12	-6	65	-66	0	18	-18			
-2	94	95	-8	37	37	-6	60	-60	H,L =	0	13	H,L =	9	13	-5	28	29	-2	8	-8			
H,L =	-8	12	-6	23	24	-6	60	-60	H,L =	0	13	H,L =	9	13	-5	28	29	-2	31	30			
-4	25	26	H,L =	0	12	-1	59	60	-3	14	15	-3	14	15	0	97	96	-2	32	-32			
-2	9	6	-2	54	-55	-2	24	-23	H,L =	1	52	H,L =	-9	14	H,L =	0	14	H,L =	8	14			
0	95	95	0	90	-90	-2	54	-55	H,L =	1	13	H,L =	-2	71	-71	-8	6	-6	-4	11	-10		
H,L =	-7	12	H,L =	1	12	H,L =	9	12	-9	28	-30	H,L =	-8	14	H,L =	0	14	H,L =	8	14			
-6	17	-16	-8	44	-46	-6	15	15	-5	56	-57	-2	12	9	-2	29	29	0	23	-24			
-4	77	-77	-6	28	29	-4	45	-47	-3	6	6	0	56	-56	0	36	-35	H,L =	-9	15			
0	26	-26	-4	45	46	-2	41	-42	-1	13	-13	H,L =	-7	14	H,L =	1	14	-1	21	-22			
H,L =	-6	12	-2	149	155	-6	56	-58	H,L =	2	13	-4	36	36	-4	91	-91	-2	54	56			
-6	22	-23	0	45	-46	H,L =	10	12	-9	39	40	-2	27	28	-6	15	-14	-3	21	21			
-4	13	14	H,L =	2	12	-2	46	-46	-7	10	-9	0	33	31	-4	29	29	-1	8	8			
-2	82	-82	-6	78	-81	H,L =	-9	13	-3	38	-39	H,L =	-6	14	-2	75	-75	H,L =	-7	15			
H,L =	-5	12	-4	51	53	-1	11	-10	-1	17	18	-6	22	-22	0	31	30	-5	15	-16			
-6	69	69	-2	19	19	H,L =	-8	13	H,L =	3	13	-4	40	-40	H,L =	2	14	-3	25	24			
-2	36	35	0	147	153	-3	28	-27	-9	25	23	-2	41	41	-8	23	-24	H,L =	-6	15			
H,L =	15	15	-4	95	-99	H,L =	-6	13	H,L =	4	13	-6	13	-13	0	28	-29	H,L =	-5	15			
-6	21	-20	-2	25	24	-9	0	-6	-4	31	-31	H,L =	3	14	-3	32	-32	-5	15	-16			
-4	92	90	H,L =	4	12	-1	7	-7	-1	17	-16	H,L =	-5	14	-2	49	49	-3	26	-26			
-8	15	15	-4	95	-99	H,L =	-6	13	H,L =	4	13	-6	13	-13	0	28	-29	H,L =	-5	15			
-6	21	-20	-2	25	24	-9	0	-6	-4	31	-31	H,L =	3	14	-3	32	-32	-5	15	-16			
-4	92	90	H,L =	4	12	-3	27	27	-5	27	28	-2	28	-28	-8	11	-11	-1	14	-12			
-2	32	32	-8	43	45	H,L =	-5	13	-1	5	-6	0	33	33	-6	44	-45	H,L =	-4	15			
0	7	3	-6	39	-41	-7	25	-25	-2	107	-109	-3	7	-8	-7	21	-22	H,L =	-4	14			
H,L =	-3	12	H,L =	5	13	-6	43	45	H,L =	-4	14	H,L =	-4	14	0	19	19	-5	19	18			

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC
-1	38	-37	H,L=	6	15	-2	28	27	-4	28	-29	-1	9	-1	-2	8	-8	-1	19	18
H,L=	-3	15	-7	35	36	-7	35	0	-2	14	-15	H,L=	4	17	0	42	41	H,L=	1	19
-5	44	44	-3	13	13	-3	13	13	-3	13	-1	H,L=	-1	16	0	74	-76	H,L=	2	18
-3	12	12	H,L=	7	15	-4	16	17	-7	19	-18	H,L=	-8	17	-3	20	-19	H,L=	2	18
-1	9	9	-5	36	38	-2	42	42	-1	28	28	H,L=	6	17	-4	36	-36	-5	26	-25
H,L=	-2	15	H,L=	6	15	0	43	40	H,L=	-7	17	-5	16	11	-2	24	22	H,L=	2	14
-7	17	-18	-1	36	-36	-1	36	16	H,L=	6	16	-1	19	-20	-3	13	16	-5	20	-19
-3	44	44	H,L=	7	15	-8	22	7	H,L=	-6	17	-1	18	-20	-3	13	16	-3	35	-34
H,L=	-1	15	-3	17	-16	-6	38	-38	-3	16	-16	H,L=	-7	18	-6	13	-12	H,L=	3	19
-5	22	-24	H,L=	8	15	-2	6	7	H,L=	-5	17	-5	11	-11	-4	11	9	H,L=	3	19
-3	26	-28	-3	21	22	0	71	69	-5	11	-11	-4	11	9	-6	30	30	-5	18	-18
-1	14	13	H,L=	-9	16	H,L=	1	16	-3	14	13	-2	20	-20	-4	7	5	-1	20	18
H,L=	0	15	0	24	-24	-4	61	-59	H,L=	-4	17	0	40	-40	-2	25	-25	H,L=	4	19
-7	20	20	H,L=	-8	16	-2	46	-39	-3	19	18	H,L=	-5	18	0	24	-23	-5	35	35
-5	33	-33	-2	65	-65	H,L=	2	16	-1	16	-15	-4	39	38	H,L=	5	18	-3	10	10
-3	56	-55	0	27	-27	-8	41	41	H,L=	-3	17	0	24	-23	-4	28	29	H,L=	5	19
-1	13	-14	H,L=	-7	16	-6	30	29	-5	27	27	H,L=	-4	18	-2	16	16	-3	30	31
H,L=	1	15	-4	9	11	-2	91	-91	-1	26	25	-2	62	61	H,L=	6	18	-1	23	23
-7	50	50	-2	58	58	0	45	-45	H,L=	-2	17	H,L=	-3	18	-2	27	27	H,L=	-5	20
H,L=	2	15	0	72	-72	H,L=	3	16	-5	25	-23	-6	44	-45	H,L=	-7	19	-2	28	27
-1	9	8	H,L=	-6	16	-6	61	60	-3	22	22	-4	11	-9	-1	16	-17	H,L=	-4	20
H,L=	1	15	-4	70	69	-4	26	26	H,L=	-1	17	-2	17	-16	H,L=	-6	19	-2	20	20
-5	29	29	-2	19	20	-2	50	50	-7	20	-20	0	76	74	-3	16	15	0	32	32
-1	42	-41	0	107	106	0	163	-103	-5	18	-17	H,L=	-2	18	H,L=	-5	19	H,L=	-3	20
H,L=	2	15	H,L=	-5	16	H,L=	4	16	-3	32	-31	-6	41	40	H,L=	-1	18	-4	20	-18
-5	62	62	-4	77	-74	-6	42	-42	H,L=	0	17	-4	53	-51	H,L=	-4	19	-2	61	58
-3	29	29	-2	39	39	-4	75	77	-7	28	27	0	65	-62	-3	7	7	0	42	40
H,L=	3	15	0	17	16	-2	29	30	-5	5	6	H,L=	-1	18	H,L=	-3	19	H,L=	-2	20
H,L=	4	15	H,L=	-4	16	0	169	169	H,L=	1	17	-4	72	68	-3	48	-48	-4	22	-20
H,L=	5	15	-6	49	-49	H,L=	5	16	-5	29	28	-2	75	-72	-1	25	23	-2	40	-38
-3	19	18	-2	120	-121	-4	85	-85	-3	43	43	0	10	11	H,L=	-2	19	0	44	41
H,L=	6	16	H,L=	-3	16	-2	57	57	-1	29	-27	H,L=	0	18	-5	13	-13	H,L=	-1	20
-7	24	-24	-6	70	70	0	37	38	H,L=	2	17	-6	41	39	-3	8	10	-4	43	-41
-5	34	-34	-4	22	-22	H,L=	6	16	-7	29	-28	-4	15	-15	-1	31	-30	-2	48	-46
-3	25	-25	-2	8	-8	-6	37	-37	-5	24	24	-2	68	65	H,L=	-1	19	0	69	-65
H,L=	5	15	0	88	-86	-4	16	-15	-1	31	29	0	56	-55	-5	41	39	H,L=	0	20
-7	22	20	H,L=	-2	16	-2	94	-96	H,L=	3	17	H,L=	1	18	-1	8	9	-4	41	39
-3	31	-33	-6	19	19	0	24	24	-5	35	-35	-6	60	-59	H,L=	0	19	-2	10	-9
-1	6	6	H,L=	7	16	-3	10	11	H,L=	7	16	-3	30	30	H,L=	0	19	-2	40	-39

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC
H,L=	1	20	H,L=	2	20	H,L=	3	20	H,L=	4	20	-1	7	-10	H,L=	-2	21
-4	35	33	-4	12	13	-4	71	-67	-2	64	-62	-3	16	16	H,L=	-1	21
-2	84	78	0	83	79	0	24	-22	H,L=	-4	21	-3	13	-13	-3	10	-7

K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC	K	FO	FC
-1	14	14	H,L=	2	21	H,L=	3	21	H,L=	4	20	-1	7	-10	H,L=	-2	21
H,L=	1	21	-3	54	-32	-1	23	-21	-2	64	-62	-3	16	16	H,L=	-1	21
-1	9	-6	-1	8	10							-1	12	-12	H,L=	0	21

DELTA G (SCALE FOR FCALC) IS -0.01288

DELTA B (OVERALL) -0.0221 (BY 2*2)

0.0119 (BY 1*1)

ATOM DEL X DEL Y DEL Z DEL B11(B) DEL B22 DEL B33 DEL B12 DEL B13 DEL B23

CA 1 1.00000 0.00000 0.00000 0.00000

SUMFO = 122853.84 SUMFC = 122853.73 SUMDF = 4222.46 R = 0.0344
(WITHOUT F0FS=0) SUMFC = 122841.53 SUMDF = 4210.27 R = 0.0343

SUM W*FO**2 = 8201258.10

SUM W*DF**2 = 16113.32

R' = 0.0020