AM-96-610

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Parameterization of energy and interactions in garnets: End-member properties

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For deposit: Tables 13 and 14

81 March-April 1996 429-447

Compressional behaviour of end-member garnets in the P range 0-300 Kbar. ΔU values (kJ/mole) arising from compressional work were obtained through gaussian integration of first order Birch EOS (BE1 in table 6) with bulk moduli of table 7.

P(kbar)	Pyrope		Almandine		Spessartine		Grossular		Uvarovite		Andradite	
	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$
0	1.00000	0.000	1.00000	0.000	1.00000	0.000	1.00000	0.000	1.00000	0.000	1.00000	0.000
10	0.99441	0.317	0.99460	0.312	0.99446	0.329	0.99408	0.371	0.99428	0.374	0.99425	0.381
20	0.98908	1.226	0.98941	1.211	0.98919	1.268	0.98844	1.431	0.98886	1.438	0.98878	1.466
30	0.98389	2.693	0.98441	2.653	0.98408	2.775	0.98292	3.158	0.98361	3.144	0.98340	3.243
40	0.97883	4.697	0.97946	4.648	0.97908	4.840	0.97761	5.487	0.97849	5.473	0.97826	5.621
50	0.97391	7.203	0.97473	7.103	0.97427	7.397	0.97246	8.385	0.97355	8.360	0.97328	8.577
60	0.96915	10.173	0.97008	10.048	0.96955	10.454	0.96750	11.794	0.96875	11.785	0.96839	12.126
70	0.96450	13.590	0.96558	13.421	0.96492	14.004	0.96261	15.769	0.96409	15.712	0.96368	16.155
80	0.96000	17.413	0.96124	17.169	0.96048	17.936	0.95788	20.201	0.95952	20.153	0.95912	20.663
90	0.95565	21.598	0.95692	21.388	0.95615	22.277	0.95335	25.014	0.95508	25.053	0.95459	25.742
100	0.95134	26.221	0.95272	25.990	0.95194	26.996	0.94889	30.305	0.95079	30.339	0.95026	31.158
110	0.94718	31.166	0.94869	30.855	0.94779	32.126	0.94454	36.010	0.94660	36.032	0.94602	37.017
120	0.94310	36.466	0.94470	36.131	0.94375	37.607	0.94029	42.113	0.94252	42.122	0.94191	43.238
130	0.93904	42.203	0.94079	41.769	0.93974	43.511	0.93615	48.568	0.93849	48.638	0.93784	49.935
140	0.93516	48.131	0.93701	47.626	0.93592	49.598	0.93212	55.367	0.93459	55.459	0.93391	56.930
150	0.93136	54.360	0.93329	53.839	0.93215	56.045	0.92813	62.594	0.93074	62.702	0.93002	64.343
160	0.92762	60.912	0.92960	60.416	0.92844	62.813	0.92430	69.994	0.92701	70.190	0.92622	72.106
170	0.92400	67.672	0.92602	67.230	0.92482	69.862	0.92051	77.804	0.92335	78.015	0.92255	80.077
180	0.92037	74.866	0.92249	74.340	0.92128	77.168	0.91679	85.939	0.91974	86.207	0.91891	88.461
190	0.91688	82.157	0.91909	81.587	0.91783	84.708	0.91317	94.326	0.91620	94.717	0.91537	97.095
200	0.91344	89.763	0.91571	89.170	0.91436	92.696	0.90968	102.810	0.91275	103.459	0.91185	106.163
210	0.91007	97.581	0.91240	96.991	0.91104	100.736	0.90615	111.873	0.90935	112.511	0.90849	115.221
220	0.90673	105.704	0.90917	104.989	0.90775	109.085	0.90274	121.040	0.90605	121.727	0.90511	124.827
230	0.90349	113.966	0.90597	113.297	0.90454	117.612	0.89942	130.370	0.90281	131.191	0.90183	134.554
240	0.90029	122.470	0.90281	121.856	0.90133	126.516	0.89612	140.077	0.89962	140.949	0.89856	144.706
250	0.89712	131.287	0.89975	130.497	0.89821	135.567	0.89287	150.042	0.89643	151.110	0.89543	154.841
260	0.89404	140.190	0.89671	139.447	0.89516	144.764	0.88968	160.239	0.89336	161.291	0.89227	165.483
270	0.89099	149.363	0.89373	148.559	0.89215	154.215	0.88658	170.539	0.89034	171.724	0.88920	176.248
280	0.88801	158.655	0.89078	157.926	0.88920	163.826	0.88354	181.039	0.88728	182.687	0.88617	187.259
290	0.88506	168.208	0.88791	167.360	0.88625	173.764	0.88055	191.725	0.88438	193.481	0.88321	198.429
300	0.88215	177.957	0.88504	177.159	0.88341	183.684	0.87759	202.679	0.88149	204.591	0.88029	209.850

P(kbar)	Knoringite		Calderite		Skiagite		Khoarite		MnCrGarnet		FeCrGarnet	
	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$	$\frac{V}{V_0}$	$-\int_{V_o}^{V} PdV$
0	1.00000	0.000	1.00000	0.000	1.00000	0.000	1.00000	0.000	1.00000	0.000	1.00000	0.000
10	0.99470	0.313	0.99452	0.343	0.99471	0.321	0.99462	0.324	0.99461	0.334	0.99477	0.314
20	0.98964	1.209	0.98933	1.317	0.98960	1.252	0.98955	1.236	0.98954	1.270	0.98980	1.209
30	0.98469	2.666	0.98426	2.894	0.98461	2.768	0.98457	2.722	0.98450	2.814	0.98491	2.669
40	0.97990	4.638	0.97929	5.056	0.97975	4.838	0.97968	4.762	0.97968	4.882	0.98014	4.670
50	0.97527	7.084	0.97450	7.742	0.97509	7.391	0.97502	7.264	0.97497	7.479	0.97555	7.141
60	0.97071	10.031	0.96982	10.947	0.97053	10.435	0.97041	10.293	0.97040	10.563	0.97107	10.089
70	0.96627	13.418	0.96525	14.646	0.96606	13.965	0.96592	13.769	0.96590	14.146	0.96668	13.500
80	0.96196	17.217	0.96085	18.762	0.96174	17.908	0.96162	17.624	0.96159	18.103	0.96244	17.304
90	0.95778	21.390	0.95660	23.255	0.95751	22.268	0.95736	21.932	0.95732	22.549	0.95828	21.532
100	0.95368	25.963	0.95237	28.248	0.95336	27.057	0.95320	26.653	0.95322	27.321	0.95418	26.181
110	0.94964	30.938	0.94828	33.589	0.94933	32.200	0.94916	31.702	0.94918	32.505	0.95027	31.089
120	0.94577	36.173	0.94426	39.328	0.94540	37.686	0.94522	37.113	0.94525	38.039	0.94640	36.413
130	0.94190	41.849	0.94034	45.427	0.94151	43.594	0.94136	42.865	0.94138	43.958	0.94257	42.133
140	0.93820	47.716	0.93650	51.863	0.93779	49.688	0.93757	48.958	0.93765	50.127	0.93889	48.058
150	0.93454	53.935	0.93277	58.602	0.93411	56.168	0.93388	55.336	0.93391	56.765	0.93523	54.410
160	0.93095	60.469	0.92908	65.714	0.93047	63.004	0.93030	61.956	0.93034	63.532	0.93165	61.042
170	0.92741	67.322	0.92546	73.147	0.92694	70.089	0.92669	69.050	0.92676	70.759	0.92823	67.779
180	0.92395	74.442	0.92197	80.730	0.92342	77.558	0.92319	76.370	0.92328	78.234	0.92477	75.021
190	0.92058	81.758	0.91854	88.632	0.92005	85.133	0.91982	83.792	0.91991	85.859	0.92144	82.395
200	0.91726	89.383	0.91513	96.908	0.91673	92.996	0.91646	91.621	0.91655	93.890	0.91811	90.144
210	0.91402	97.188	0.91177	105.470	0.91343	101.207	0.91319	99.608	0.91327	102.137	0.91485	98.143
220	0.91076	105.418	0.90851	114.201	0.91019	109.678	0.90992	107.999	0.91003	110.696	0.91173	106.184
230	0.90764	113.685	0.90533	123.125	0.90705	118.267	0.90679	116.410	0.90690	119.319	0.90859	114.626
240	0.90455	122.230	0.90214	132.480	0.90391	127.218	0.90362	125.313	0.90380	128.281	0.90552	123.267
250	0.90151	130.998	0.89905	141.919	0.90088	136.266	0.90057	134.235	0.90071	137.569	0.90250	132.142
260	0.89853	139.938	0.89601	151.592	0.89786	145.625	0.89757	143.399	0.89769	147.031	0.89951	141.257
270	0.89554	149.256	0.89298	161.609	0.89489	155.205	0.89460	152.797	0.89476	156.589	0.89662	150.451
280	0.89263	158.686	0.89009	171.505	0.89198	164.957	0.89166	162.484	0.89189	166.289	0.89374	159.952
290	0.88977	168.307	0.88713	182.041	0.88908	175.023	0.88876	172.373	0.88898	176.488	0.89090	169.666
300	0.88701	177.908	0.88431	192.465	0.88629	185.028	0.88597	182.238	0.88615	186.760	0.88813	179.483

Calculated static energy differences (U_P-U_0; kJ/mole) of end-member garnets for various values of the hardness factor ρ (Å)

P(kbar)	Pyrope		Almandine		Spessartine		Grossular		Uvarovite		Andradite	
	0.480	0.490	0.450	0.460	0.450	0.460	0.480	0.490	0.500	0.510	0.480	0.490
0	0	0	0	0	0	0	0	0	0	0	0	0
10	-1.125	-2.875	-1.875	-3.875	-1.129	-3.172	-3.234	-5.18	-1.676	-3.383	0.121	-1.687
20	2.812	-0.75	0	-4.062	2.051	-1.992	2.649	-1.195	0.941	-2.418	1.84	-1.738
30	2.375	-2.938	0.437	-5.625	3.668	-2.355	3.098	-2.668	2.675	-2.328	3.367	-1.996
40	4.812	-2.188	1.875	-6.187	5.5	-2.523	8.141	0.496	6.105	-0.543	7.418	0.305
50	8.625	-0.125	6.562	-3.437	9.719	-0.254	10.805	1.281	8.496	0.215	10.188	1.332
60	14.125	3.625	12.25	0.313	14.707	2.758	18.613	7.238	14.308	4.402	15.738	5.141
70	15.625	3.5	14.75	0.813	18.156	4.242	22.891	9.644	20.086	8.574	21.867	9.547
80	22.628	8.812	18.25	2.375	22.457	6.602	30.59	15.496	25.367	12.25	26.59	12.555
90	30.441	14.937	24.187	6.375	30.672	12.895	39.903	23.008	30.82	16.094	33.52	17.754
100	35.535	18.347	30.062	10.313	37.047	17.363	47.613	28.891	39.187	22.887	40.961	23.492
110	40.562	21.714	33.937	12.313	44.363	22.762	58.004	37.469	47.55	29.672	49.606	30.442
120	48.109	27.617	43.375	19.813	52.617	29.109	65.153	42.797	58.39	38.953	57.879	37.035
130	54.73	32.558	49.562	24.125	60.348	34.906	76.172	52.035	63.965	42.953	66.977	44.442
140	62.906	39.097	57.562	30.313	68.746	41.445	88.383	62.465	75.902	53.328	76.195	51.981
150	73.578	48.152	65	35.813	79.977	50.797	95.641	67.91	84.882	60.758	87.043	61.164
160	81.242	54.191	74.375	43.25	88.73	57.672	110.231	80.75	93.769	68.101	98.195	70.633
170	91.5	62.855	82.605	49.688	97.082	64.141	120.86	89.605	106.933	79.722	108.52	79.305
180	100.652	70.371	91.664	56.875	108.934	74.141	132.563	99.531	117.55	88.789	121.109	90.239
190	109.543	77.664	101.535	64.938	118.902	82.254	145.289	110.492	129.047	98.746	132.082	99.551
200	122.019	88.543	111.402	72.938	127.25	88.719	159.125	122.609	142.914	111.086	142.852	108.653
210	130.335	95.273	121.843	81.563	141.281	100.922	171.625	133.34	152.902	119.539	158.402	122.594
220	139.023	102.367	131.039	88.863	152.699	110.5	184.977	144.957	166.437	131.578	169.649	132.176
230	152.214	113.972	143.402	99.383	163.367	119.34	199.793	158.039	178.351	141.976	183.277	144.172
240	166.046	126.222	152.925	107.074	175.91	130.031	212.758	169.277	192.062	154.183	197.203	156.449
250	176.425	135.007	163.906	116.234	187.691	139.973	228.176	182.961	206.047	166.644	211.004	168.629
260	188.082	145.101	178.152	128.648	200.363	150.828	243.063	196.105	218.59	177.676	224.512	180.504
270	201.543	156.996	189.414	138.102	213.422	162.059	258.301	209.641	234.293	191.883	240.719	195.082
280	210.437	164.339	199.746	146.606	227.102	173.922	274.539	224.164	248.316	204.387	252.945	205.676
290	223.429	175.757	213.558	158.629	239.098	184.094	289.637	237.57	262.179	216.769	268.637	219.758
300	237.019	187.781	224.882	168.129	255.18	198.387	305.238	251.465	277.058	230.14	284.098	233.578

P(kbar)	Knoringite		Calderite		Skiagite		Khoharite		MnCrGarnet		FeCrGarnet	
	0.500	0.510	0.460	0.470	0.460	0.470	0.480	0.490	0.470	0.480	0.470	0.480
0	0	0	0	0	0	0	0	0	0	0	0	0
10	-0.879	-2.399	-3.395	-5.227	-0.602	-2.394	-2.344	-3.973	-0.426	-2.214	-2.25	-4.024
20	0.547	-2.454	-2.477	-6.094	0.636	-2.934	-1.406	-4.625	3.785	0.266	0.98	-2.512
30	0.067	-4.418	-0.368	-5.762	3.003	-2.328	0.047	-4.758	5.894	0.61	1.707	-3.508
40	1.41	-4.547	1.878	-5.301	3.953	-3.16	1.465	-4.938	10.16	3.149	4.207	-2.746
50	5.551	-1.852	3.964	-4.977	6.796	-2.062	6.477	-1.477	13.836	5.102	8.644	-0.016
60	7.309	-1.555	9.273	-1.438	9.109	-1.488	11.024	1.492	17.652	7.196	13.715	3.371
70	11.348	1.027	11.136	-1.34	12.531	0.191	13.434	2.332	22.578	10.387	17.23	5.179
80	17.094	5.343	17.398	3.187	17.343	3.277	17.059	4.425	28.781	14.914	21.379	7.656
90	19.493	6.32	24.222	8.297	19.957	4.164	23.25	9.074	34.426	18.852	28.777	13.379
100	22.985	8.39	29.812	12.144	26.914	9.398	28.469	12.753	44.84	27.594	34.902	17.828
110	30.637	14.613	36.66	17.273	31.671	12.441	36.102	18.851	49.652	30.727	39.957	21.226
120	36.586	19.167	42.734	21.633	39	18.078	42.266	23.496	58.84	38.243	48.398	28.019
130	42.598	23.761	50.203	27.375	45.625	22.988	47.375	27.093	65.734	43.461	56.18	34.133
140	51.801	31.585	58.289	33.758	54.933	30.629	56.629	34.835	77.082	53.161	64.398	40.734
150	60.176	38.574	67.386	41.164	61.652	35.668	65.906	42.605	83.535	57.942	69.348	44.011
160	67.231	44.242	75.789	47.855	69.203	41.531	74.192	49.414	94.898	67.68	81.078	54.109
170	75.633	51.246	86.386	56.758	79.425	50.074	82.082	55.785	105.164	76.282	90.953	62.39
180	82.207	56.449	96.941	65.636	84.882	53.836	90.027	62.222	114.457	83.926	98.648	68.453
190	91.934	64.816	107.398	74.437	94.906	62.211	99.262	69.984	126.832	94.676	108.301	76.488
200	100.192	71.695	117.812	83.14	105.636	71.285	110.016	79.25	137.652	103.856	119.644	86.203
210	111.489	81.64	128.058	91.699	116.851	80.836	121.817	89.585	149.074	113.653	127.992	92.926
220	121.094	89.855	139.75	101.722	124	86.305	130.606	96.875	158.933	121.883	140.055	103.398
230	131.082	98.507	151.804	112.117	137.984	98.656	143.402	108.218	170.777	132.114	151.473	113.215
240	140.567	106.636	162.214	120.847	147.679	106.684	152.996	116.32	184.242	143.961	161.933	122.07
250	152.391	117.105	174.472	131.433	158.093	115.461	165.383	127.257	196.265	154.364	173.055	131.586
260	164.278	127.656	186.019	141.332	169.132	124.848	176.66	137.074	209.488	165.957	184.672	141.601
270	174.965	136.98	199.46	153.086	180.679	134.742	188.457	147.41	221.758	176.625	197.121	152.469
280	184.11	144.785	212.496	164.508	191.898	144.336	199.02	156.488	237.98	191.258	207.957	161.719
290	196.055	155.386	226.089	176.422	204.523	155.301	209.699	165.707	249.738	201.407	221.355	173.523
300	208.981	166.996	238.992	187.687	216.437	165.582	224.531	179.109	265.445	215.493	236.508	187.105