

## Solution-Phase Structural Characterization of an Array of Inorganic $\text{Ga}_{13-x}\text{In}_x$ ( $0 \leq x \leq 6$ ) Nanoscale Clusters by $^1\text{H-NMR}$ and QMC.

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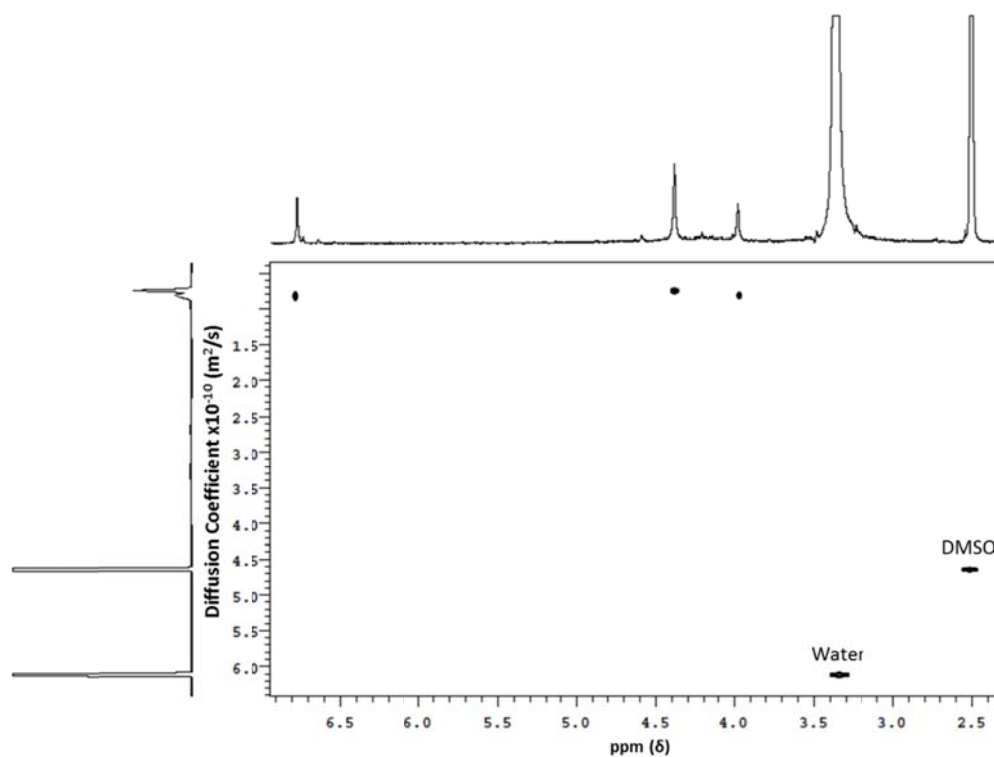


Figure S1: Representative DOSY of 2 mM  $\text{Ga}_7\text{In}_6$  in  $d_6$ -DMSO.

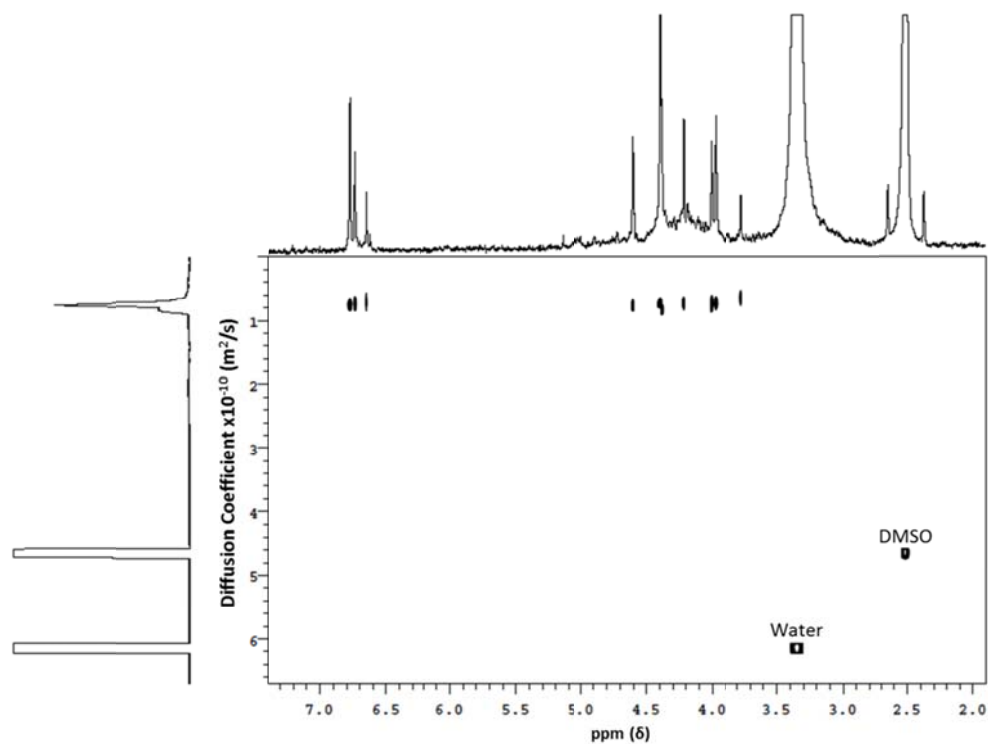


Figure S2: Representative DOSY of 2 mM  $\text{Ga}_8\text{In}_5$  in  $d_6$ -DMSO.

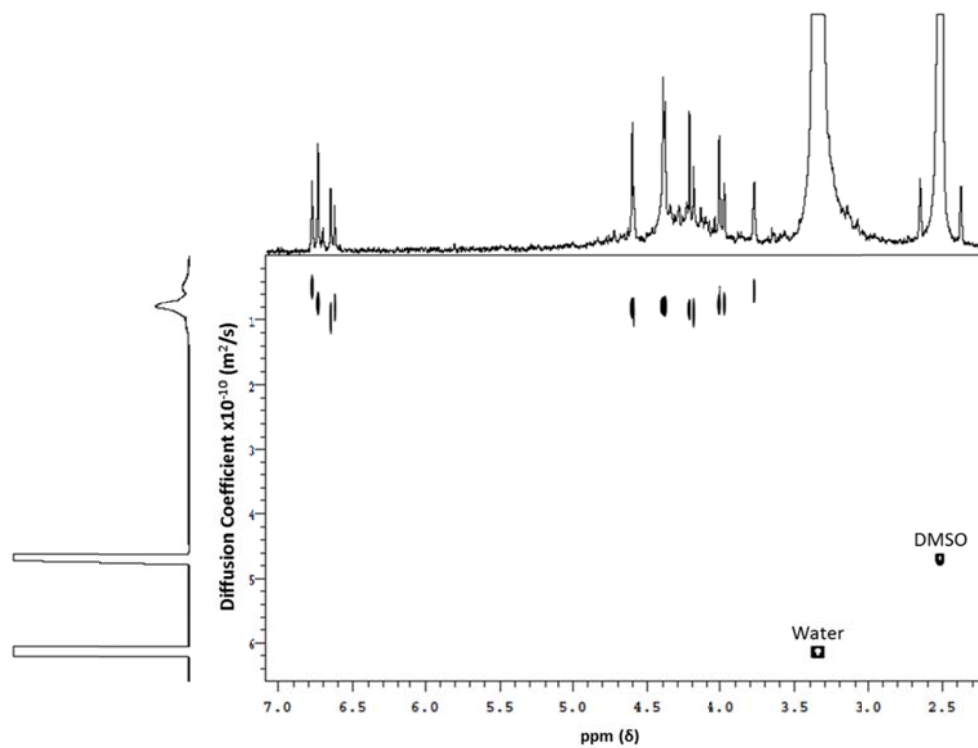


Figure S3: Representative DOSY of 2 mM  $\text{Ga}_9\text{In}_4$  in  $d_6$ -DMSO.

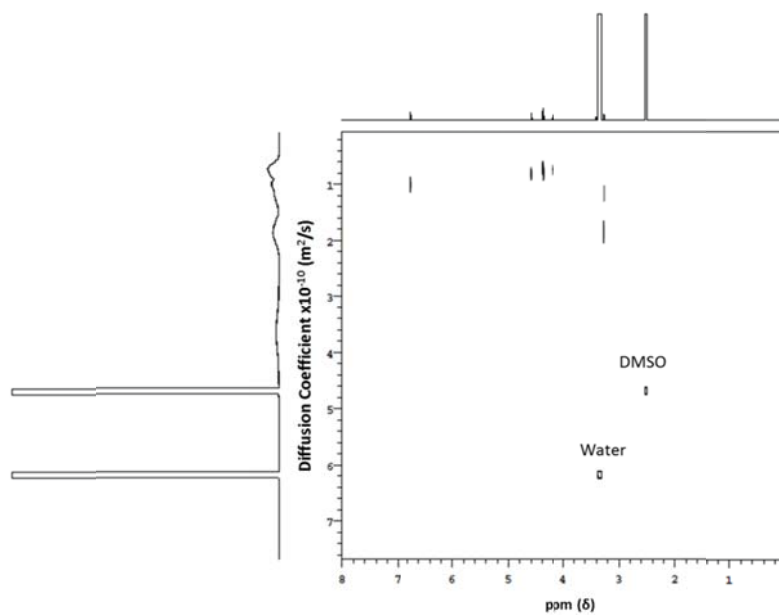


Figure S4: Representative DOSY of 2 mM  $\text{Ga}_{10}\text{In}_3$  in  $d_6$ -DMSO.

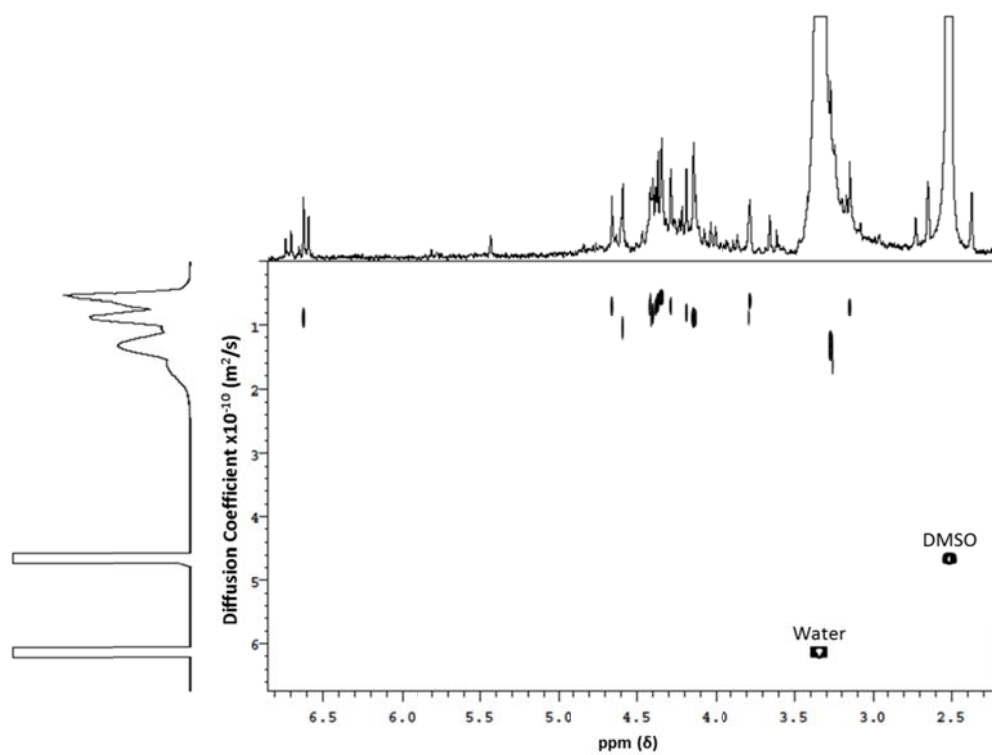


Figure S5: Representative DOSY of 2 mM Ga<sub>11</sub>In<sub>2</sub> in *d*<sub>6</sub>-DMSO.

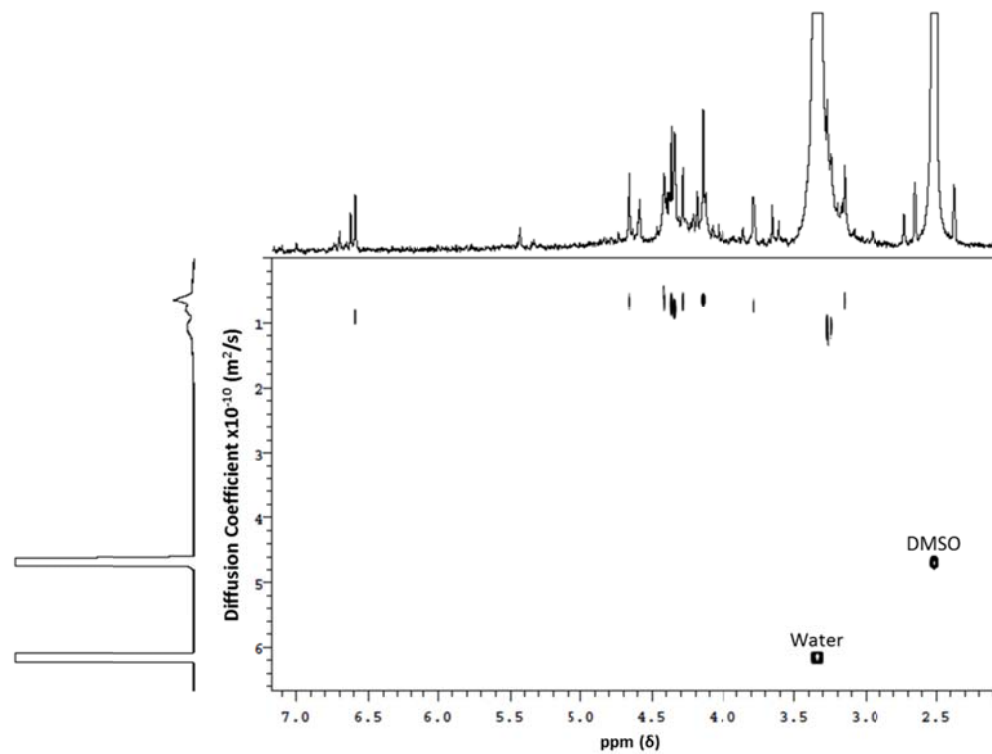


Figure S6: Representative DOSY of 2 mM Ga<sub>12</sub>In<sub>1</sub> in *d*<sub>6</sub>-DMSO.

**Table S1:** Diffusion Data and Radii of Ga<sub>13-x</sub>In<sub>x</sub> Clusters. T = 298 K;  $\eta = 2.03 \times 10^{-3}$  Pa·s; Concentration = 2 mM; Solvent *d*<sub>6</sub>-DMSO; 500 MHz NMR

Species	Average Diffusion Coefficient x 10 <sup>-10</sup> (m <sup>2</sup> /s)	Average Radius (Å)
Ga <sub>7</sub> In <sub>6</sub>	0.99 ± 0.12	11.1 ± 1.1
Ga <sub>8</sub> In <sub>5</sub>	1.16 ± 0.04	9.4 ± 0.4
Ga <sub>9</sub> In <sub>4</sub>	0.92 ± 0.11	11.7 ± 1.5
Ga <sub>10</sub> In <sub>3</sub>	1.09 ± 0.17	9.9 ± 1.6
Ga <sub>11</sub> In <sub>2</sub>	0.97 ± 0.13	11.1 ± 1.4
Ga <sub>12</sub> In <sub>1</sub>	0.90 ± 0.14	12.0 ± 1.9
Ga <sub>13</sub>	0.96 ± 0.06	11.2 ± 0.8

Initially, the clusters of interest were optimized with full quantum mechanics, as described in the manuscript, as implemented in Gaussian03. The computed shifts were then scaled with constant scaling factors (F) for each type of proton and plotted against the experimental results. These results look uncannily good, with nearly all peaks accounted for. However, these predictions switch the ordering of the internal and external  $\mu_2$ -OH protons.

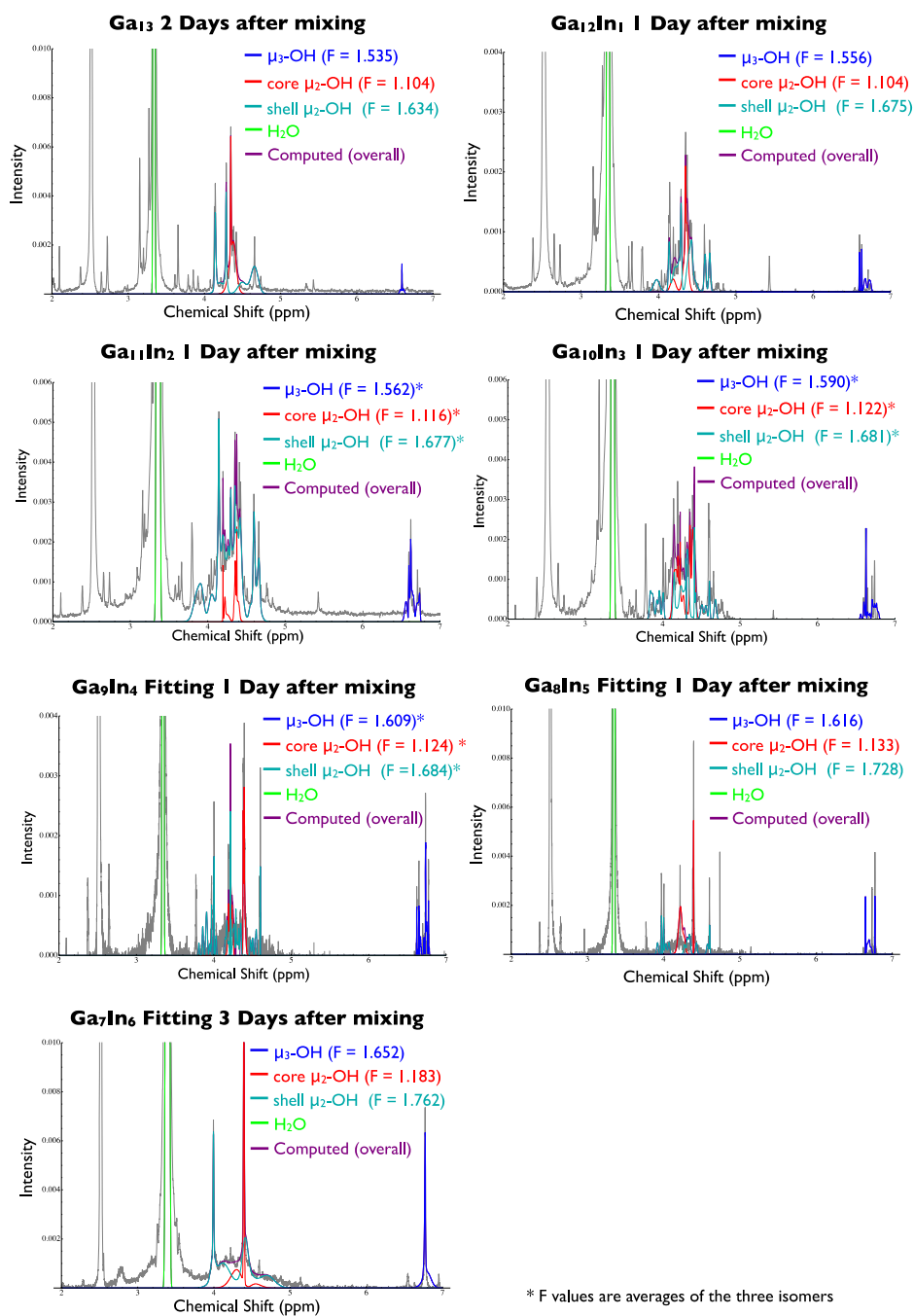


Figure S7: Experimental vs. computed spectra for quantum mechanically optimized cluster structures without counterions.

XYZ of Ga<sub>7</sub>In<sub>6</sub>

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In	4.916147	1.984595	-1.232080
In	-5.565192	-2.143545	0.821920
In	-4.355745	3.298356	-2.468080
In	3.705700	-3.457305	2.056920
In	-0.835464	-5.457933	-2.100080
In	0.185419	5.298983	1.689920
Ga	-0.325023	-0.078975	-0.205080
Ga	2.752941	-0.523227	0.135920
Ga	-3.403986	0.365278	-0.546080
Ga	-1.472784	2.825119	-0.393080
Ga	0.821739	-2.983069	-0.016080
Ga	-2.228224	-2.536819	-0.561080
Ga	1.578179	2.377869	0.150920
O	4.164989	0.066657	-1.007080
O	-4.815035	-0.224606	0.596920
O	-2.406718	3.634196	-1.850080
O	1.755673	-3.792145	1.439920
O	-2.173335	-3.887823	-1.911080
O	1.523290	3.727874	1.500920
O	3.098222	2.903744	-0.870080
O	-3.748267	-3.062694	0.459920
O	-4.358908	1.311356	-1.896080
O	3.707863	-1.469306	1.486920
O	0.747622	-4.411063	-1.277080
O	-1.398667	4.252113	0.867920
O	6.855085	1.226436	-1.763080
O	-7.506130	-1.384386	1.351920
O	3.863536	-5.454318	2.836920
O	1.656518	6.508863	2.685920
O	5.730309	3.962528	-1.455080
O	-6.381354	-4.121478	1.045920
O	5.736726	-3.149472	2.693920
O	-1.173445	6.956095	1.884920
O	1.373028	0.542886	-0.958080
O	-2.022074	-0.702835	0.547920
O	-1.502934	0.996122	-1.341080
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O	-5.251194	-2.162571	2.944920
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H	7.613133	1.816374	-1.783080
H	4.114090	1.290661	-3.775080
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H	3.210482	-6.116265	2.597920
H	4.587518	-5.684378	3.424920
H	2.535693	-3.550209	4.548920

H 3.462806 -2.171286 4.481920

XYZ of Ga<sub>8</sub>In<sub>5</sub>

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In	4.873787	2.031745	-1.197722
In	-5.537755	-2.329641	0.725042
In	-4.417078	3.213365	-2.424610
In	3.752112	-3.511254	1.950928
In	0.079189	5.188439	1.793958
Ga	-0.332493	-0.148457	-0.236329
Ga	2.752062	-0.547103	0.101465
Ga	-3.418047	0.250171	-0.574125
Ga	-1.530739	2.738874	-0.354598
Ga	0.864751	-3.035831	-0.117062
Ga	-2.191401	-2.629585	-0.658668
Ga	1.526433	2.331672	0.185986
O	4.155990	0.095900	-1.022736
O	-4.820975	-0.392814	0.550079
O	-2.475600	3.567719	-1.793326
O	1.809615	-3.864651	1.320667
O	-2.109839	-3.945162	-2.041900
O	1.444889	3.646249	1.569193
O	3.039200	2.909530	-0.817574
O	-3.704168	-3.207444	0.344892
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O	6.826903	1.321231	-1.742473
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O	1.355986	0.521745	-0.969108
O	-2.019936	-0.820641	0.496404
O	-1.526667	0.933963	-1.348138
O	0.862699	-1.231859	0.875459
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O	-0.238845	1.490209	0.832281
O	2.620118	1.075107	1.110155
O	-3.285086	-1.373020	-1.582837
O	-3.084794	1.876399	0.359649
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O	-0.892841	-3.502917	0.446605
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O	-3.827294	2.787007	-4.443657
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O	-4.633010	-5.339229	-4.310019
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O	-5.472232	-0.531432	-3.840194
O	-3.934709	4.321321	2.331707
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N	6.607123	-2.457070	-1.874682
N	-1.264649	6.909212	-2.582210
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N	-4.394333	3.391855	3.010633
N	3.728350	-3.688762	-3.484292
N	-2.185423	-5.233516	2.971234
N	1.521455	4.935620	-3.443913
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O	2.884794	-4.895186	7.070987
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O	5.639415	-2.249536	-1.130340
O	-1.158178	6.011440	-1.734211
O	4.617826	1.554929	5.041749
O	-5.283794	-1.852860	-5.514433
O	-5.362041	3.599390	3.754974

O	4.697073	-3.897303	-4.227656
O	-2.079968	-6.130281	3.818255
O	1.414983	5.833367	-4.290912
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O	6.787310	-0.454643	1.548976
O	-4.215151	5.394215	6.436288
O	7.143905	0.421060	-4.528228
N	-7.879671	-1.753288	4.758693
N	3.418297	-5.585265	6.155557
N	7.767988	-0.905766	0.912592
N	-3.233470	4.943135	5.798906
N	7.214688	1.456399	-5.232350
O	-8.583557	-2.689461	4.415598
O	4.627489	-5.749912	6.105033
O	8.186077	-2.029546	1.135404
O	-2.814364	3.818372	6.021695
O	7.919589	2.391565	-4.888278
H	2.638767	1.043016	1.845623
H	-3.303754	-1.339956	-2.317281
H	-3.238997	1.951826	1.075432
H	2.573029	-2.249757	-1.548116
H	-1.053462	-3.631469	1.153259
H	0.388477	3.334555	-1.625916
H	4.529565	-0.437819	-1.102329
H	-5.195550	0.140887	0.629669
H	-2.180613	4.151325	-1.840076
H	1.514645	-4.449256	1.367391
H	-2.734777	-3.982181	-2.239244
H	2.069792	3.685267	1.766587
H	1.427616	0.582103	-1.611644
H	-2.092602	-0.879018	1.138987
H	-1.460911	0.930279	-1.994292
H	0.795928	-1.227168	1.520636
H	-0.301831	-1.765990	-1.942341
H	-0.364134	1.468084	1.468656
H	2.870297	3.479003	-1.223796
H	-3.536284	-3.775960	0.752136
H	-4.693469	0.759984	-2.368677
H	4.029481	-1.056906	1.897022
H	1.458625	-4.501637	-1.735024
H	-2.123575	4.202724	1.262317
O	-4.608320	5.226226	-3.154809
O	-5.274502	4.051918	-0.632883
O	-6.441996	2.885976	-3.072404
O	-2.190590	-6.696445	-3.297425
O	-1.472402	-6.539966	-0.533074
O	0.644056	-7.114011	-2.498501

O	6.518429	1.507596	-6.285907
H	-4.146357	1.992954	-4.879386
H	-3.244492	3.389169	-4.910452
H	-6.791354	1.993700	-3.122538
H	-6.996483	3.632613	-3.311968
H	-5.333960	5.458243	-3.738750
H	-3.967529	5.893294	-2.896622
H	-5.967608	3.580886	-0.166041
H	-4.962083	4.898500	-0.301885
H	-1.953825	-7.364132	-0.638805
H	-1.314856	-6.185023	0.345441
H	0.317913	-8.009356	-2.609681
H	1.589213	-6.943546	-2.492180
H	-2.371822	-7.589573	-2.996106
H	-2.654840	-6.343356	-4.058822
H	-0.431119	-5.421374	-5.003200
H	0.312825	-4.071301	-4.380557
H	-5.562541	-3.136344	3.358604
H	-4.754531	-1.685699	3.285687
H	-8.239486	-2.221594	1.273075
H	-7.618583	-0.697910	1.508680
H	-7.014903	-4.622063	0.305259
H	-5.972797	-4.921491	1.565410
H	-6.894081	-3.070400	-1.566184
H	-6.215246	-1.579786	-1.847446
H	1.990854	6.046460	3.586168
H	1.707841	7.292726	2.521452
H	-2.253181	6.645650	2.019501
H	-0.984898	7.712407	2.137019
H	-0.978810	3.774369	3.907897
H	-0.234863	5.124467	4.529541
H	0.649886	5.887085	-0.817123
H	1.288857	7.066218	0.166123
H	5.548279	1.281837	1.374758
H	6.228111	2.772444	1.094499
H	5.304808	4.624474	-2.036075
H	6.349937	4.324174	-0.778941
H	6.953615	0.399996	-1.981362
H	7.574501	1.924680	-1.745732
H	4.089565	1.387811	-3.759368
H	4.897573	2.838430	-3.831286
H	6.330496	-3.929569	2.840308
H	6.125367	-2.290656	2.650878
H	4.299078	-5.194405	-0.169742
H	5.303601	-3.876833	-0.304589
H	3.302561	-6.191207	2.423940
H	4.669995	-5.756114	3.265070
H	2.578527	-3.687075	4.436768
H	3.481390	-2.290868	4.406704

Ga -0.744157 -5.486353 -2.266640



XYZ of Ga<sub>9</sub>In<sub>4</sub>O

193

In	5.02800	1.71500	-1.15100
In	-5.61100	-2.08000	0.72800
In	-4.17800	3.34700	-2.49500
In	0.37200	5.15900	1.74000
Ga	-0.29200	-0.18200	-0.21100
Ga	2.76500	-0.73200	0.16600
Ga	-3.34900	0.36700	-0.58800
Ga	-1.34000	2.76000	-0.38700
Ga	0.75600	-3.12500	-0.03400
Ga	-2.27000	-2.57200	-0.61500
Ga	1.68700	2.20600	0.19200
O	4.21100	-0.17900	-0.95300
O	-4.79400	-0.18600	0.53100
O	-2.22700	3.61200	-1.84800
O	1.64300	-3.97700	1.42600
O	-2.24200	-3.91200	-1.97600
O	1.65900	3.54500	1.55400
O	3.23700	2.69000	-0.80400
O	-3.82000	-3.05600	0.38200
O	-4.25400	1.35600	-1.94100
O	3.67000	-1.72100	1.52000
O	0.65100	-4.53800	-1.30900
O	-1.23500	4.17200	0.88800
O	6.94800	0.89700	-1.66400
O	-7.53200	-1.26200	1.24000
O	3.67600	-5.72100	2.83500
O	1.86900	6.31000	2.76700
O	5.91100	3.66600	-1.34500
O	-6.49500	-4.03200	0.92300
O	5.62600	-3.47900	2.73800
O	-0.93400	6.85800	1.93300
O	1.43600	0.38900	-0.93600
O	-2.01800	-0.75600	0.51400
O	-1.41800	0.94100	-1.35200
O	0.83600	-1.30700	0.93000
O	-0.45800	-1.83100	-1.25600
O	-0.12500	1.46600	0.83300
O	2.70600	0.91100	1.14800
O	-3.28900	-1.27700	-1.57000
O	-2.94300	1.98900	0.32400
O	2.35900	-2.35500	-0.74700
O	-1.02900	-3.49300	0.51800
O	0.44700	3.12700	-0.94000
O	5.83800	1.70100	0.84700
O	-6.42100	-2.06600	-1.26800

O	4.42700	-4.62300	0.30400
O	1.17000	6.14600	-0.00200
O	4.74200	1.76300	-3.27700
O	-5.32600	-2.12900	2.85500
O	-3.59000	2.85900	-4.50100
O	3.00600	-3.22500	4.07700
O	-0.34600	-4.98100	-4.14800
O	-0.23800	4.61600	3.72500
O	-4.81100	-5.21200	-4.24900
O	7.05000	-1.97300	-2.42900
O	-1.68100	6.79800	-3.58300
O	4.82500	-0.00400	3.44100
O	-5.40800	-0.36100	-3.86300
O	-3.68600	4.50500	2.24900
O	3.10300	-4.87100	-2.67100
O	-3.27500	-5.19100	2.14800
O	2.69200	4.82500	-2.57000
O	4.22800	4.84700	3.82800
N	-5.48000	-4.43300	-3.55500
N	6.53700	-2.86700	-1.73900
N	-0.83900	6.87500	-2.67600
N	4.15500	0.77500	4.13400
N	-4.73900	-1.14100	-4.55700
N	-4.19900	3.61200	2.93700
N	3.61500	-3.97600	-3.36000
N	-2.43300	-5.11500	3.05500
N	1.85100	4.74900	-3.47700
N	4.89600	4.06700	3.13400
O	-6.67800	-4.20400	-3.79700
O	6.95800	-4.03600	-1.76300
O	-0.03300	7.81700	-2.60700
O	2.95800	1.00500	3.89300
O	-3.54200	-1.37000	-4.31600
O	-3.77900	2.44200	2.91400
O	3.19600	-2.80800	-3.33700
O	-1.62800	-4.17100	3.12400
O	1.04400	3.80600	-3.54600
O	6.09400	3.83900	3.37500
O	-7.27700	-1.39100	5.79000
O	2.60700	-4.96900	7.20300
O	8.34300	-0.62200	0.17500
O	-2.39300	5.85600	4.85100
O	-4.94800	-3.85600	-2.59700
O	5.57400	-2.59900	-1.00900
O	-0.78700	5.98700	-1.81300
O	4.68700	1.35200	5.09200
O	-5.27100	-1.71700	-5.51500
O	-5.16200	3.88000	3.66800
O	4.57900	-4.24600	-4.09000

O	-2.38200	-6.00200	3.91700
O	1.79900	5.63700	-4.33900
O	4.36500	3.49100	2.17600
O	-7.83000	-0.30300	4.00900
O	2.35200	-6.17200	5.42700
O	6.78500	-0.82200	1.65400
O	-3.95200	5.65700	6.33300
O	7.24600	-0.06300	-4.43100
N	-7.96000	-1.32100	4.72700
N	3.11400	-5.70000	6.30400
N	7.74800	-1.33200	1.03600
N	-2.98800	5.14600	5.71300
N	7.37700	0.95600	-5.15100
O	-8.70700	-2.22600	4.39100
O	4.31400	-5.92600	6.26900
O	8.10600	-2.47200	1.28000
O	-2.62900	4.00500	5.95800
O	8.12500	1.86000	-4.81400
H	2.71600	0.89000	1.88400
H	-3.29900	-1.25400	-2.30500
H	-3.10000	2.08400	1.03700
H	2.51600	-2.45000	-1.45900
H	-1.20300	-3.60100	1.22500
H	0.62000	3.23700	-1.64700
H	4.55800	-0.73200	-1.02100
H	-5.14200	0.36800	0.59800
H	-1.90200	4.18000	-1.90100
H	1.31800	-4.54500	1.47900
H	-2.86600	-3.92100	-2.18000
H	2.28300	3.55600	1.75800
H	1.51700	0.43600	-1.57900
H	-2.10000	-0.80000	1.15700
H	-1.34600	0.92400	-1.99800
H	0.76300	-1.28900	1.57400
H	-0.32700	-1.82700	-1.89100
H	-0.25700	1.46100	1.46800
H	3.10200	3.26100	-1.22100
H	-3.68600	-3.62600	0.79900
H	-4.57900	0.91200	-2.40400
H	3.99700	-1.27700	1.98200
H	1.29000	-4.64500	-1.62300
H	-1.87300	4.27800	1.20100
O	-4.25900	5.35500	-3.25800
O	-5.00900	4.25700	-0.72500
O	-6.21000	3.11300	-3.15900
O	-2.45100	-6.67600	-3.19000
O	-1.75300	-6.51200	-0.42100
O	0.35100	-7.22400	-2.35400
O	6.69400	1.02600	-6.21200

H	-3.94500	2.07500	-4.92700
H	-2.97300	3.42300	-4.97000
H	-6.60400	2.23900	-3.19900
H	-6.72300	3.88300	-3.41600
H	-4.96600	5.61400	-3.85300
H	-3.58700	5.99300	-3.00300
H	-5.72900	3.82900	-0.25900
H	-4.65700	5.09200	-0.40400
H	-2.27500	-7.31200	-0.51900
H	-1.58600	-6.15100	0.45400
H	-0.02000	-8.10300	-2.45500
H	1.30300	-7.10200	-2.34100
H	-2.68100	-7.55300	-2.87700
H	-2.88900	-6.31200	-3.96200
H	-0.61200	-5.51900	-4.89600
H	0.19400	-4.19900	-4.28700
H	-5.70200	-2.84200	3.37400
H	-4.82100	-1.43600	3.28700
H	-8.30800	-1.82600	1.24600
H	-7.61300	-0.33300	1.46400
H	-7.19800	-4.30100	0.32900
H	-6.18500	-4.63300	1.60400
H	-6.98000	-2.78800	-1.56500
H	-6.22300	-1.33800	-1.86200
H	2.30700	5.94700	3.53900
H	2.09800	7.18900	2.45200
H	-1.88500	6.73600	1.91800
H	-0.56500	7.73900	2.03300
H	-0.77800	3.83400	3.86500
H	0.02800	5.15500	4.47300
H	1.00300	5.78500	-0.87500
H	1.69200	6.94600	0.09700
H	5.63800	0.97300	1.44000
H	6.39600	2.42200	1.14400
H	5.59900	4.26800	-2.02500
H	6.61500	3.93500	-0.75200
H	7.03000	-0.03300	-1.88700
H	7.72500	1.46100	-1.66800
H	4.23800	1.07000	-3.71000
H	5.11900	2.47700	-3.79600
H	6.13900	-4.24800	2.99500
H	6.02000	-2.60400	2.77800
H	4.07600	-5.45600	-0.01700
H	5.14700	-4.19300	-0.16200
H	3.00400	-6.35900	2.58100
H	4.38400	-5.98000	3.43000
H	2.38900	-3.78900	4.54700
H	3.36200	-2.44100	4.50500
Ga	-0.95500	-5.52400	-2.16300

Ga 3.59400 -3.71300 2.07100

XYZ of Ga<sub>9</sub>In<sub>4</sub>m

193

In	-5.36900	-2.52400	0.76900
In	-4.50500	3.04200	-2.42100
In	3.97200	-3.31300	1.92200
In	-0.05900	5.22600	1.74800
Ga	-0.26600	-0.13500	-0.24900
Ga	2.83500	-0.40400	0.06500
Ga	-3.36900	0.13400	-0.56300
Ga	-1.58400	2.70000	-0.37300
Ga	1.05000	-2.96900	-0.12400
Ga	-2.02400	-2.69300	-0.64200
Ga	1.49200	2.42300	0.14400
O	4.20100	0.29000	-1.07500
O	-4.73400	-0.56000	0.57700
O	-2.57400	3.48000	-1.80800
O	2.04100	-3.75000	1.31000
O	-1.90000	-4.01200	-2.01800
O	1.36700	3.74100	1.52100
O	2.97100	3.05700	-0.87600
O	-3.50400	-3.32700	0.37800
O	-4.38700	1.04800	-1.88800
O	3.85300	-1.31800	1.39100
O	1.05100	-4.37500	-1.41200
O	-1.58500	4.10400	0.91600
O	6.81300	1.62100	-1.82400
O	-7.34700	-1.89100	1.32500
O	4.25200	-5.31200	2.66200
O	1.34500	6.50100	2.75900
O	5.53200	4.28000	-1.45500
O	-6.06600	-4.55000	0.95900
O	5.98600	-2.89800	2.55300
O	-1.51200	6.79700	1.98400
O	1.38700	0.60000	-1.00000
O	-1.91800	-0.87200	0.50200
O	-1.51400	0.89100	-1.35600
O	0.98200	-1.16100	0.85900
O	-0.30100	-1.78200	-1.30900
O	-0.23200	1.51300	0.81000
O	2.64400	1.21800	1.06600
O	-3.17700	-1.48800	-1.56300
O	-3.09500	1.77800	0.35900
O	2.56100	-2.04900	-0.85800
O	-0.68200	-3.50500	0.45700
O	0.15000	3.23500	-0.95500
O	5.68300	2.29600	0.71600
O	-6.21600	-2.56600	-1.21200

O	4.84900	-4.12600	0.13000
O	0.61000	6.29900	0.00300
O	4.50600	2.29500	-3.38700
O	-5.03900	-2.56500	2.88900
O	-3.91400	2.62900	-4.44200
O	3.38100	-2.89900	3.94400
O	0.04400	-4.88100	-4.23600
O	-0.57800	4.61200	3.73800
O	-4.38200	-5.52300	-4.25700
O	7.16400	-1.22000	-2.62200
O	-2.35800	6.71900	-3.51800
O	4.88300	0.48200	3.30900
O	-5.41500	-0.75100	-3.80700
O	-4.02900	4.19700	2.32500
O	3.49700	-4.46800	-2.82300
O	-2.73000	-5.41900	2.11000
O	2.19700	5.14800	-2.60800
O	3.84900	5.25200	3.76100
N	-5.10600	-4.81500	-3.54200
N	6.74900	-2.16400	-1.93300
N	-1.50900	6.86400	-2.62600
N	4.15700	1.18800	4.02300
N	-4.69100	-1.45900	-4.52200
N	-4.44400	3.25300	3.01300
N	3.91100	-3.52300	-3.51200
N	-1.88100	-5.27300	3.00200
N	1.34900	5.00300	-3.50000
N	4.57300	4.54400	3.04600
O	-6.32500	-4.69500	-3.75900
O	7.27500	-3.28900	-1.97800
O	-0.79200	7.87600	-2.56100
O	2.94000	1.30900	3.80700
O	-3.47300	-1.57900	-4.30600
O	-3.91900	2.12800	2.97000
O	3.38600	-2.39900	-3.46700
O	-1.16500	-4.26100	3.06700
O	0.63100	3.99000	-3.56400
O	5.79100	4.42500	3.26200
O	-6.99300	-2.03700	5.86800
O	3.20500	-4.70100	7.05700
O	8.37800	0.22000	-0.02900
O	-2.81500	5.63700	4.91800
O	-4.61100	-4.20100	-2.58800
O	5.78000	-1.99200	-1.18200
O	-1.35900	5.97700	-1.77400
O	4.65300	1.80300	4.97800
O	-5.18600	-2.07300	-5.47500
O	-5.41400	3.42500	3.76400
O	4.88100	-3.69600	-4.26200

O	-1.73100	-6.16000	3.85300
O	1.19800	5.89000	-4.35100
O	4.07800	3.93000	2.09100
O	-7.67800	-0.98900	4.10900
O	3.02700	-5.90700	5.27400
O	6.87400	-0.13600	1.47800
O	-4.32000	5.28200	6.42600
O	7.14400	0.71800	-4.60700
N	-7.69900	-2.02100	4.81900
N	3.75900	-5.37400	6.14100
N	7.86800	-0.55000	0.83500
N	-3.32600	4.86800	5.78300
N	7.16600	1.75200	-5.31700
O	-8.36700	-2.98800	4.48700
O	4.97300	-5.48900	6.08100
O	8.33400	-1.65400	1.06100
O	-2.85900	3.76300	6.00800
O	7.83500	2.71700	-4.98500
H	2.67000	1.19100	1.80100
H	-3.20300	-1.46000	-2.29800
H	-3.24600	1.85100	1.07600
H	2.71300	-2.12200	-1.57400
H	-0.83100	-3.63600	1.16600
H	0.29800	3.36700	-1.66400
H	4.59600	-0.22800	-1.15400
H	-5.13000	-0.04200	0.65700
H	-2.30400	4.07500	-1.86100
H	1.77000	-4.34600	1.36300
H	-2.52400	-4.07600	-2.21000
H	1.99100	3.80700	1.71200
H	1.45100	0.66000	-1.64300
H	-1.98300	-0.92900	1.14500
H	-1.45300	0.88600	-2.00300
H	0.92000	-1.15600	1.50400
H	-0.18300	-1.76000	-1.94600
H	-0.35100	1.48900	1.44700
H	2.77500	3.61600	-1.28300
H	-3.30900	-3.88600	0.78700
H	-4.67900	0.58000	-2.34900
H	4.14700	-0.84900	1.85200
H	1.69100	-4.41900	-1.73900
H	-2.22400	4.14700	1.24100
O	-4.78500	5.04100	-3.16000
O	-5.38100	3.85500	-0.62700
O	-6.52000	2.62800	-3.05000
O	-1.87700	-6.77200	-3.25800
O	-1.14300	-6.57000	-0.50100
O	0.97900	-7.06700	-2.48100
O	6.46000	1.76800	-6.36500



H	-4.20400	1.82000	-4.87100
H	-3.36100	3.25200	-4.91700
H	-6.83200	1.72100	-3.09200
H	-7.10600	3.34900	-3.28900
H	-5.52500	5.24000	-3.74000
H	-4.17000	5.73600	-2.91100
H	-6.05000	3.35900	-0.15100
H	-5.10100	4.71600	-0.30300
H	-1.59100	-7.41400	-0.59800
H	-0.99300	-6.20300	0.37500
H	0.68900	-7.97600	-2.58400
H	1.91600	-6.85800	-2.48300
H	-2.01900	-7.67000	-2.95000
H	-2.36200	-6.44300	-4.01700
H	-0.18600	-5.43500	-4.98500
H	0.50700	-4.05200	-4.37700
H	-5.33800	-3.31500	3.40700
H	-4.59200	-1.83300	3.31900
H	-8.06800	-2.52400	1.33900
H	-7.50900	-0.97500	1.56100
H	-6.75300	-4.87800	0.37400
H	-5.68900	-5.12600	1.62700
H	-6.71200	-3.33300	-1.50700
H	-6.09800	-1.81800	-1.80200
H	1.83000	6.17300	3.52000
H	1.48700	7.40000	2.45000
H	-2.44800	6.58700	1.98600
H	-1.22400	7.70600	2.08700
H	-1.04000	3.78200	3.87900
H	-0.34800	5.16600	4.48700
H	0.46000	5.93300	-0.87100
H	1.05800	7.14300	0.10000
H	5.56300	1.54700	1.30400
H	6.17800	3.06300	1.01000
H	5.15300	4.85700	-2.12300
H	6.22000	4.60700	-0.87300
H	6.97600	0.70400	-2.05900
H	7.53500	2.25500	-1.83700
H	4.05900	1.56200	-3.81800
H	4.80600	3.04500	-3.90400
H	6.57300	-3.61900	2.79200
H	6.29800	-1.99100	2.59500
H	4.57100	-4.98400	-0.19400
H	5.51800	-3.62700	-0.34400
H	3.63800	-6.00600	2.41400
H	4.99300	-5.51000	3.24100
H	2.82700	-3.52200	4.41900
H	3.67100	-2.09000	4.37300
Ga	-0.47300	-5.49700	-2.24600

Ga 4.83700 2.25300 -1.26600

XYZ of Ga<sub>9</sub>In<sub>4</sub>p

193

In	4.87200	2.13000	-1.12800
In	-5.53400	-2.28600	0.69800
In	-4.42000	3.32500	-2.33200
In	3.75800	-3.48000	1.90100
Ga	-0.33100	-0.07700	-0.21500
Ga	2.75400	-0.47900	0.11500
Ga	-3.41700	0.32400	-0.54500
Ga	-1.53400	2.81000	-0.27200
Ga	0.87000	-2.96500	-0.15700
Ga	-2.18700	-2.55200	-0.69100
Ga	1.52400	2.39600	0.26100
O	4.15700	0.19000	-0.99500
O	-4.82000	-0.34500	0.56500
O	-2.47900	3.66800	-1.69300
O	1.81600	-3.82300	1.26300
O	-2.10300	-3.83700	-2.10200
O	1.44000	3.68000	1.67200
O	3.03600	2.99700	-0.73000
O	-3.69900	-3.15300	0.30000
O	-4.38700	1.31300	-1.85300
O	3.72300	-1.46800	1.42400
O	0.82600	-4.33400	-1.48300
O	-1.49000	4.17800	1.05400
O	6.82600	1.43400	-1.68800
O	-7.49000	-1.58900	1.25700
O	3.95200	-5.50800	2.58800
O	1.51800	6.40500	2.98500
O	5.64900	4.13100	-1.25700
O	-6.31200	-4.28700	0.82800
O	5.78100	-3.16400	2.55800
O	-1.31800	6.83600	2.19600
O	1.35600	0.61100	-0.93300
O	-2.01800	-0.76800	0.50300
O	-1.52700	1.02700	-1.30400
O	0.86500	-1.18300	0.87400
O	-0.42200	-1.69300	-1.31900
O	-0.24000	1.53800	0.88800
O	2.61900	1.12100	1.15800
O	-3.28200	-1.27700	-1.58800
O	-3.08700	1.93000	0.42400
O	2.42300	-2.08600	-0.85500
O	-0.88700	-3.44700	0.39600
O	0.22500	3.29100	-0.82600
O	5.70200	2.08600	0.86100
O	-6.36400	-2.24100	-1.28900

O	4.61800	-4.27900	0.09400
O	0.79900	6.30700	0.21900
O	4.56200	2.24200	-3.24900
O	-5.22400	-2.39800	2.81900
O	-3.83000	2.94200	-4.35900
O	3.16600	-3.09800	3.92800
O	-0.17600	-4.72400	-4.32800
O	-0.48800	4.56900	3.89700
O	-4.62400	-5.18600	-4.40000
O	7.07000	-1.39600	-2.56100
O	-2.11900	6.94000	-3.31200
O	4.80700	0.23600	3.39700
O	-5.47000	-0.39100	-3.82700
O	-3.94000	4.33100	2.44700
O	3.27800	-4.48700	-2.87700
O	-3.02400	-5.32000	1.98100
O	2.36200	5.16400	-2.41100
O	3.96100	5.03000	3.97100
N	-5.32600	-4.46900	-3.67100
N	6.61200	-2.34100	-1.90100
N	-1.27300	7.02700	-2.41000
N	4.10400	0.95200	4.12500
N	-4.76800	-1.10700	-4.55600
N	-4.39900	3.38700	3.10600
N	3.73500	-3.54200	-3.53700
N	-2.17800	-5.23300	2.88300
N	1.51600	5.07700	-3.31300
N	4.66200	4.31300	3.24200
O	-6.53600	-4.29500	-3.89400
O	7.09300	-3.48500	-1.97200
O	-0.51700	8.00700	-2.31200
O	2.89400	1.12700	3.90300
O	-3.55800	-1.28200	-4.33400
O	-3.91800	2.24300	3.03600
O	3.25500	-2.39900	-3.46600
O	-1.42200	-4.25200	2.98000
O	0.75900	4.09600	-3.41000
O	5.87300	4.14000	3.46400
O	-7.18100	-1.87200	5.79600
O	2.89100	-4.97500	6.99000
O	8.31800	-0.07600	0.08000
O	-2.69200	5.65100	5.08700
O	-4.81400	-3.90100	-2.69700
O	5.64400	-2.15000	-1.15200
O	-1.16600	6.11200	-1.58100
O	4.61600	1.52000	5.09900
O	-5.27900	-1.67600	-5.52900
O	-5.36700	3.57700	3.85500
O	4.70400	-3.73300	-4.28400

O	-2.07100	-6.14700	3.71000
O	1.40800	5.99200	-4.14000
O	4.15200	3.74500	2.26800
O	-7.80900	-0.75000	4.06200
O	2.68100	-6.12400	5.17300
O	6.78900	-0.41200	1.56500
O	-4.22300	5.31600	6.57400
O	7.14500	0.59400	-4.49200
N	-7.87700	-1.80000	4.74300
N	3.42600	-5.64400	6.06000
N	7.77000	-0.84800	0.91900
N	-3.24100	4.88000	5.92700
N	7.21400	1.64500	-5.17400
O	-8.58000	-2.72900	4.38000
O	4.63600	-5.80600	6.00600
O	8.19000	-1.97500	1.11800
O	-2.82000	3.75100	6.12600
O	7.91800	2.57300	-4.81000
H	2.63800	1.07300	1.89300
H	-3.30000	-1.22800	-2.32200
H	-3.24100	1.99000	1.14100
H	2.57700	-2.14600	-1.57100
H	-1.04800	-3.59000	1.10000
H	0.38500	3.43600	-1.53000
H	4.53100	-0.34100	-1.08600
H	-5.19500	0.18600	0.65600
H	-2.18500	4.25300	-1.72700
H	1.52200	-4.40900	1.29700
H	-2.72800	-3.87100	-2.30000
H	2.06500	3.71600	1.87000
H	1.42800	0.68500	-1.57400
H	-2.09100	-0.84000	1.14400
H	-1.46100	1.03700	-1.95000
H	0.79800	-1.19200	1.51900
H	-0.29800	-1.65800	-1.95500
H	-0.36600	1.50200	1.52400
H	2.86600	3.57500	-1.12400
H	-3.53000	-3.73000	0.69500
H	-4.69300	0.87000	-2.32800
H	4.03200	-1.02500	1.89900
H	1.46600	-4.39500	-1.80600
H	-2.12900	4.23800	1.37600
O	-4.61400	5.35200	-3.01900
O	-5.27900	4.12300	-0.52300
O	-6.44500	3.00800	-2.98700
O	-2.17900	-6.56100	-3.41600
O	-1.46200	-6.46300	-0.64900
O	0.65600	-6.99200	-2.62500
O	6.51800	1.71700	-6.22600

H	-4.14700	2.15700	-4.81200
H	-3.24800	3.55500	-4.81300
H	-6.79300	2.11700	-3.05600
H	-7.00000	3.75900	-3.21000
H	-5.34000	5.59600	-3.59800
H	-3.97500	6.01500	-2.74600
H	-5.97200	3.64100	-0.06600
H	-4.96800	4.96300	-0.17400
H	-1.94200	-7.28500	-0.77200
H	-1.30500	-6.12600	0.23700
H	0.33100	-7.88500	-2.75600
H	1.60100	-6.82000	-2.61500
H	-2.35900	-7.46100	-3.13400
H	-2.64400	-6.19300	-4.17000
H	-0.42200	-5.24700	-5.09400
H	0.32000	-3.91000	-4.44200
H	-5.55800	-3.14900	3.31400
H	-4.75200	-1.69600	3.27200
H	-8.23600	-2.19400	1.24800
H	-7.61700	-0.67500	1.51600
H	-7.00700	-4.57100	0.22900
H	-5.96500	-4.89600	1.48300
H	-6.88800	-2.98000	-1.60800
H	-6.21200	-1.48200	-1.85800
H	1.98200	6.03800	3.74000
H	1.69800	7.30600	2.70200
H	-2.26200	6.66400	2.18500
H	-0.99500	7.73000	2.32600
H	-0.98400	3.75500	4.01200
H	-0.24200	5.09200	4.66300
H	0.64200	5.97100	-0.66600
H	1.28000	7.12900	0.34200
H	5.54700	1.32600	1.42800
H	6.22500	2.82400	1.17900
H	5.29900	4.74100	-1.91100
H	6.34500	4.41500	-0.66000
H	6.95400	0.51900	-1.94600
H	7.57300	2.03900	-1.67800
H	4.08900	1.54000	-3.70300
H	4.89500	2.99300	-3.74400
H	6.33700	-3.91400	2.78200
H	6.12900	-2.27200	2.62700
H	4.30700	-5.11700	-0.25500
H	5.31000	-3.79500	-0.36200
H	3.31200	-6.17000	2.31600
H	4.67900	-5.75200	3.16700
H	2.58400	-3.71100	4.38200
H	3.48500	-2.31300	4.38200
Ga	-0.73500	-5.37100	-2.35900

Ga 0.07200 5.21500 1.92900

XYZ of Ga<sub>10</sub>In<sub>3</sub>a

193

In	-5.459691	-2.255648	0.770072
In	-4.253182	3.204908	-2.489959
In	0.262171	5.201813	1.697833
Ga	-0.221729	-0.169244	-0.223520
Ga	2.856090	-0.604881	0.129677
Ga	-3.300549	0.266390	-0.576722
Ga	-1.378234	2.731868	-0.403826
Ga	0.933771	-3.070364	-0.042218
Ga	-2.115118	-2.631722	-0.599273
Ga	1.671663	2.292234	0.152229
O	4.271414	-0.005229	-1.004152
O	-4.714872	-0.333259	0.557113
O	-2.308138	3.544391	-1.861486
O	1.863680	-3.882882	1.414441
O	-2.049548	-3.976470	-1.955031
O	1.606096	3.635982	1.507982
O	3.194631	2.827687	-0.859392
O	-3.638086	-3.167175	0.412347
O	-4.252388	1.215363	-1.926868
O	3.807925	-1.553859	1.480823
O	0.870182	-4.492924	-1.309917
O	-1.314642	4.153428	0.863868
O	6.961096	1.166784	-1.742551
O	-7.405550	-1.505271	1.294506
O	3.970599	-5.544352	2.813700
O	1.724660	6.412052	2.706003
O	5.825854	3.897748	-1.427513
O	-6.270314	-4.237243	0.981464
O	5.836776	-3.232730	2.689641
O	-1.103060	6.853548	1.893972
O	1.477694	0.461577	-0.965896
O	-1.920146	-0.802062	0.518852
O	-1.397965	0.907051	-1.360121
O	0.955510	-1.246536	0.913082
O	-0.336628	-1.828009	-1.259509
O	-0.106826	1.489526	0.811469
O	2.745313	1.039428	1.104563
O	-3.188769	-1.378916	-1.551608
O	-2.945964	1.906533	0.324282
O	2.501514	-2.246020	-0.772331
O	-0.831498	-3.500620	0.526752
O	0.389043	3.161135	-0.973791
O	5.842988	1.941933	0.773840
O	-6.286451	-2.280425	-1.219879
O	4.659754	-4.431745	0.271805



O	1.009029	6.209079	-0.055253
O	4.711936	1.943673	-3.341435
O	-5.155391	-2.283161	2.894391
O	-3.665384	2.728779	-4.498435
O	3.220934	-3.068266	4.050386
O	-0.133215	-4.985533	-4.137796
O	-0.311239	4.647046	3.689751
O	-4.587729	-5.380659	-4.200039
O	7.161781	-1.701245	-2.495508
O	-1.893309	6.739620	-3.615284
O	4.915491	0.214241	3.383882
O	-5.358949	-0.552729	-3.830922
O	-3.764845	4.403344	2.243757
O	3.321390	-4.742832	-2.690802
O	-3.000482	-5.272065	2.183873
O	2.557027	4.932577	-2.630918
O	4.144270	5.041167	3.753995
N	-5.279383	-4.622996	-3.503805
N	6.687475	-2.609911	-1.797748
N	-1.047801	6.851334	-2.715879
N	4.222845	0.970906	4.079107
N	-4.667295	-1.310392	-4.527156
N	-4.239146	3.494682	2.940517
N	3.794692	-3.833169	-3.388561
N	-2.153974	-5.160348	3.083283
N	1.711518	4.820863	-3.530323
N	4.834923	4.283500	3.057756
O	-6.486921	-4.438856	-3.736533
O	7.150289	-3.763334	-1.819795
O	-0.276175	7.822584	-2.657976
O	3.016299	1.156044	3.847388
O	-3.460753	-1.494531	-4.295433
O	-3.776337	2.341254	2.919470
O	3.332882	-2.680743	-3.366514
O	-1.383351	-4.188101	3.141186
O	0.938896	3.848610	-3.588235
O	6.042462	4.100365	3.289489
O	-7.108198	-1.602642	5.842530
O	2.912063	-4.810313	7.187218
O	8.426352	-0.291697	0.090679
O	-2.500269	5.812896	4.828944
O	-4.760688	-4.022562	-2.552709
O	5.721300	-2.373328	-1.060112
O	-0.955962	5.969744	-1.849393
O	4.741540	1.571340	5.030203
O	-5.185995	-1.910831	-5.477252
O	-5.205321	3.731265	3.678153
O	4.761866	-4.070753	-4.125197
O	-2.063134	-6.040937	3.948769

O	1.619675	5.702449	-4.395809
O	4.317228	3.683069	2.106665
O	-7.715395	-0.544627	4.061448
O	2.686129	-6.031161	5.419668
O	6.889240	-0.540347	1.584531
O	-4.038391	5.564234	6.324791
O	7.270940	0.205135	-4.508497
N	-7.801463	-1.563157	4.785499
N	3.437520	-5.526603	6.287402
N	7.864670	-1.018409	0.959856
N	-3.061955	5.086180	5.699121
N	7.358009	1.224674	-5.233539
O	-8.517978	-2.496032	4.460016
O	4.644331	-5.709507	6.243126
O	8.266152	-2.143232	1.206661
O	-2.659471	3.960360	5.945927
O	8.075522	2.156547	-4.907056
H	2.761976	1.022191	1.840578
H	-3.205439	-1.360684	-2.286618
H	-3.100553	1.998844	1.038001
H	2.656098	-2.338336	-1.485050
H	-0.995409	-3.612319	1.235512
H	0.551951	3.273831	-1.682552
H	4.637468	-0.545751	-1.071896
H	-5.081926	0.207260	0.624852
H	-2.004723	4.122640	-1.919499
H	1.560268	-4.462131	1.472450
H	-2.674542	-4.008605	-2.153051
H	2.231084	3.670117	1.706012
H	1.551513	0.507693	-1.609364
H	-1.994972	-0.846181	1.162324
H	-1.330929	0.889155	-2.005907
H	0.887476	-1.227638	1.557867
H	-0.210712	-1.821757	-1.895916
H	-0.233738	1.482271	1.447867
H	3.034747	3.391048	-1.277608
H	-3.479210	-3.729544	0.831564
H	-4.564813	0.757391	-2.384367
H	4.122350	-1.095881	1.938331
H	1.509932	-4.577434	-1.628362
H	-1.953384	4.236946	1.181314
O	-4.414050	5.204869	-3.261745
O	-5.102214	4.092255	-0.717845
O	-6.281236	2.893235	-3.135690
O	-2.167110	-6.751532	-3.154043
O	-1.452484	-6.548567	-0.391791
O	0.659600	-7.193041	-2.340016
O	6.664739	1.264154	-6.289570
H	-3.994889	1.930580	-4.918538

H	-3.073049	3.312838	-4.976103
H	-6.643239	2.005197	-3.168338
H	-6.824471	3.642635	-3.391831
H	-5.135080	5.435180	-3.852037
H	-3.764303	5.867879	-3.015780
H	-5.802964	3.640861	-0.243080
H	-4.778384	4.940910	-0.403544
H	-1.945447	-7.367771	-0.481733
H	-1.291689	-6.177937	0.479628
H	0.320893	-8.085731	-2.433578
H	1.607087	-7.035998	-2.334957
H	-2.361745	-7.635601	-2.834896
H	-2.624675	-6.407565	-3.923618
H	-0.386020	-5.537034	-4.881446
H	0.375901	-4.185218	-4.284869
H	-5.501491	-3.007639	3.419562
H	-4.672629	-1.570487	3.318815
H	-8.160727	-2.097787	1.309379
H	-7.518545	-0.578608	1.515148
H	-6.968661	-4.534879	0.393907
H	-5.933566	-4.823208	1.662397
H	-6.821741	-3.023876	-1.508680
H	-6.121036	-1.549202	-1.818852
H	2.182216	6.069081	3.476583
H	1.919296	7.297125	2.385860
H	-2.049542	6.696514	1.887918
H	-0.766351	7.747236	1.986529
H	-0.820359	3.846727	3.837825
H	-0.058434	5.198548	4.433402
H	0.848230	5.838445	-0.925672
H	1.501991	7.028283	0.034688
H	5.675581	1.209707	1.371798
H	6.377281	2.684380	1.062631
H	5.487098	4.484701	-2.107451
H	6.525210	4.195395	-0.841952
H	7.075089	0.239120	-1.962192
H	7.717269	1.759299	-1.756419
H	4.229178	1.231004	-3.766859
H	5.058035	2.668151	-3.866606
H	6.380008	-3.981131	2.945786
H	6.198776	-2.343693	2.722293
H	4.336917	-5.278396	-0.042482
H	5.360493	-3.978355	-0.201951
H	3.320847	-6.207367	2.568736
H	4.692629	-5.774661	3.403997
H	2.628598	-3.652325	4.528054
H	3.551434	-2.270068	4.471494
Ga	-0.705626	-5.541301	-2.144878
Ga	3.809731	-3.544392	2.041915

Ga 5.017236 1.916163 -1.217112

XYZ of Ga<sub>10</sub>In<sub>3</sub>b

193

In	5.022072	1.839058	-1.085373
In	-5.592574	-2.065968	0.703195
In	-4.193561	3.437829	-2.403592
Ga	-0.285738	-0.112942	-0.191081
Ga	2.774308	-0.649721	0.177004
Ga	-3.346784	0.423864	-0.559179
Ga	-1.353562	2.825259	-0.305924
Ga	0.781073	-3.051146	-0.075251
Ga	-2.248066	-2.506997	-0.646792
Ga	1.676564	2.280115	0.264601
O	4.217381	-0.063910	-0.928735
O	-4.788857	-0.161974	0.546574
O	-2.245212	3.702506	-1.749906
O	1.672737	-3.928363	1.367732
O	-2.209950	-3.817843	-2.036381
O	1.638422	3.589961	1.654159
O	3.224177	2.795405	-0.719720
O	-3.795679	-3.022288	0.337529
O	-4.257294	1.435352	-1.892334
O	3.684805	-1.661238	1.511160
O	0.686954	-4.438127	-1.379938
O	-1.259470	4.211241	0.998732
O	6.947557	1.045396	-1.613437
O	-7.520018	-1.271222	1.230264
O	3.716078	-5.687733	2.741372
O	1.828464	6.329534	2.924789
O	5.891297	3.800221	-1.237354
O	-6.463813	-4.027106	0.856149
O	5.651375	-3.430762	2.693311
O	-0.977150	6.876443	2.100333
O	1.438574	0.485429	-0.902274
O	-2.009104	-0.713338	0.520065
O	-1.418734	1.027022	-1.309387
O	0.848231	-1.253931	0.927209
O	-0.440340	-1.740354	-1.270713
O	-0.131122	1.514501	0.887552
O	2.703484	0.971592	1.193251
O	-3.274987	-1.198474	-1.575442
O	-2.951908	2.028939	0.387086
O	2.379421	-2.255765	-0.770290
O	-1.001460	-3.442678	0.467242
O	0.430958	3.215768	-0.849420
O	5.829623	1.788879	0.912566
O	-6.401112	-2.014793	-1.293728
O	4.461751	-4.531401	0.235194

O	1.132886	6.219126	0.153176
O	4.737550	1.930274	-3.210801
O	-5.309053	-2.157157	2.828609
O	-3.601505	2.996009	-4.418646
O	3.029018	-3.222835	4.035442
O	-0.304259	-4.827594	-4.228126
O	-0.268202	4.601768	3.844953
O	-4.767794	-5.087068	-4.338701
O	7.069717	-1.807081	-2.438825
O	-1.719032	6.927830	-3.416582
O	4.826762	0.023348	3.468866
O	-5.398238	-0.249232	-3.851027
O	-3.713900	4.499087	2.363636
O	3.142398	-4.725970	-2.745827
O	-3.237619	-5.190178	2.059222
O	2.666117	4.963296	-2.441414
O	4.196278	4.860155	3.957509
N	-5.443030	-4.327111	-3.628980
N	6.562063	-2.718717	-1.768965
N	-0.878995	6.990970	-2.507382
N	4.150514	0.782363	4.177543
N	-4.723002	-1.009189	-4.560747
N	-4.221541	3.587480	3.032497
N	3.649079	-3.813307	-3.415671
N	-2.396582	-5.127065	2.968436
N	1.826080	4.900155	-3.350614
N	4.870514	4.100225	3.247775
O	-6.642323	-4.100882	-3.867171
O	6.990492	-3.884569	-1.816978
O	-0.079348	7.936807	-2.417695
O	2.952234	1.009535	3.940396
O	-3.524695	-1.235361	-4.323569
O	-3.793126	2.421598	2.985483
O	3.221624	-2.648481	-3.367675
O	-1.597908	-4.180202	3.058139
O	1.025406	3.953346	-3.440344
O	6.069847	3.875025	3.484997
O	-7.268126	-1.494256	5.776605
O	2.639143	-5.034814	7.123252
O	8.351550	-0.503025	0.193791
O	-2.432054	5.803173	4.995253
O	-4.915568	-3.767147	-2.658221
O	5.596528	-2.472255	-1.033728
O	-0.821547	6.085057	-1.663312
O	4.677977	1.342327	5.148303
O	-5.250478	-1.569182	-5.530508
O	-5.187075	3.833943	3.767734
O	4.615573	-4.060825	-4.149925
O	-2.340094	-6.031922	3.811523

O	1.768618	5.806039	-4.193684
O	4.344052	3.540235	2.277029
O	-7.826895	-0.373091	4.018452
O	2.393428	-6.202527	5.322747
O	6.793848	-0.743697	1.667485
O	-3.990784	5.562467	6.470933
O	7.254393	0.146235	-4.400657
N	-7.950019	-1.406838	4.715065
N	3.151394	-5.743211	6.209678
N	7.760385	-1.234629	1.038981
N	-3.023233	5.071539	5.841442
N	7.378557	1.180985	-5.098225
O	-8.690943	-2.309112	4.359365
O	4.352580	-5.961069	6.170994
O	8.125856	-2.376966	1.259937
O	-2.656789	3.928175	6.062381
O	8.120440	2.082202	-4.741543
H	2.712762	0.934965	1.928686
H	-3.284251	-1.160878	-2.309847
H	-3.110328	2.107489	1.101611
H	2.537826	-2.334344	-1.483816
H	-1.175229	-3.567573	1.171437
H	0.603754	3.341689	-1.553598
H	4.567784	-0.613261	-1.007350
H	-5.140260	0.387404	0.625175
H	-1.924175	4.272683	-1.790296
H	1.351674	-4.499539	1.408092
H	-2.833750	-3.826102	-2.240507
H	2.262275	3.600219	1.858346
H	1.519733	0.545820	-1.543673
H	-2.091208	-0.771703	1.161512
H	-1.346242	1.023712	-1.954822
H	0.774780	-1.249566	1.571662
H	-0.308365	-1.721542	-1.905642
H	-0.264123	1.494716	1.522438
H	3.085055	3.373869	-1.124528
H	-3.657545	-3.599755	0.743353
H	-4.578945	0.998869	-2.364220
H	4.008455	-1.224809	1.983072
H	1.326844	-4.533600	-1.694986
H	-1.898372	4.305718	1.312764
O	-4.287566	5.460881	-3.124563
O	-5.032268	4.304461	-0.616373
O	-6.223890	3.203876	-3.074516
O	-2.398953	-6.556413	-3.307967
O	-1.704388	-6.446008	-0.535367
O	0.405634	-7.103356	-2.481525
O	6.696650	1.268372	-6.158766
H	-3.950713	2.219116	-4.862125

H	-2.987603	3.574096	-4.875913
H	-6.611871	2.328239	-3.133293
H	-6.742144	3.975580	-3.315759
H	-4.995878	5.727822	-3.714825
H	-3.620676	6.097548	-2.855927
H	-5.750552	3.862265	-0.159493
H	-4.686241	5.134658	-0.277396
H	-2.220678	-7.247461	-0.650751
H	-1.540755	-6.102877	0.346720
H	0.041368	-7.982776	-2.601116
H	1.357291	-6.975014	-2.464289
H	-2.622809	-7.442145	-3.013546
H	-2.838870	-6.179212	-4.072243
H	-0.566437	-5.351975	-4.987974
H	0.229824	-4.039412	-4.350022
H	-5.681466	-2.884165	3.331823
H	-4.809251	-1.470435	3.275498
H	-8.292620	-1.840984	1.223295
H	-7.607407	-0.347557	1.473904
H	-7.165207	-4.288451	0.255115
H	-6.151037	-4.640213	1.524502
H	-6.955598	-2.734173	-1.606292
H	-6.208406	-1.273723	-1.872086
H	2.268393	5.953301	3.690095
H	2.052361	7.216295	2.629400
H	-1.927793	6.748104	2.082111
H	-0.614842	7.756947	2.218928
H	-0.802299	3.813556	3.967847
H	-0.006024	5.126148	4.604800
H	0.969239	5.875965	-0.727912
H	1.649176	7.020579	0.268560
H	5.634905	1.046894	1.489868
H	6.383082	2.507288	1.225087
H	5.576535	4.414350	-1.904704
H	6.593719	4.061598	-0.638306
H	7.035905	0.120675	-1.856096
H	7.721144	1.615100	-1.605456
H	4.237762	1.243582	-3.658689
H	5.109964	2.657282	-3.714014
H	6.169655	-4.201467	2.934584
H	6.039381	-2.554126	2.752118
H	4.116777	-5.359626	-0.103709
H	5.180075	-4.087237	-0.220626
H	3.049174	-6.324431	2.473735
H	4.425390	-5.954702	3.331648
H	2.415115	-3.800921	4.492708
H	3.379211	-2.445999	4.479933
Ga	-0.911535	-5.416927	-2.255271
Ga	3.622072	-3.664682	2.020401



Ga 0.340033 5.190044 1.873080

XYZ Ga<sub>10</sub>In<sub>3</sub>c

193

In	-5.576068	-2.145786	0.689759
In	3.682516	-3.464435	2.009006
In	0.168016	5.293495	1.626113
Ga	-0.325990	-0.080625	-0.284069
Ga	2.748532	-0.526366	0.084889
Ga	-3.401512	0.365116	-0.653037
Ga	-1.471214	2.824137	-0.477152
Ga	0.818225	-2.985389	-0.089996
Ga	-2.226386	-2.537261	-0.662678
Ga	1.574406	2.375010	0.094538
O	4.171376	0.065364	-1.043678
O	-4.823356	-0.226615	0.475540
O	-2.391252	3.636300	-1.941259
O	1.738272	-3.797550	1.373111
O	-2.159187	-3.885648	-2.014736
O	1.507207	3.722398	1.446594
O	3.104081	2.902465	-0.911148
O	-3.756061	-3.064716	0.343007
O	-4.343506	1.314078	-2.010077
O	3.690517	-1.475330	1.442929
O	0.755570	-4.410905	-1.354417
O	-1.408559	4.248653	0.787267
O	6.868727	1.225892	-1.772177
O	-7.521697	-1.387140	1.203029
O	3.832538	-5.463006	2.786556
O	1.630020	6.501038	2.638211
O	5.741798	3.961681	-1.469395
O	-6.394788	-4.123933	0.902245
O	5.707560	-3.158388	2.665608
O	-1.192201	6.950588	1.811603
O	1.379198	0.542245	-1.019912
O	-2.030178	-0.705496	0.451779
O	-1.492937	0.996998	-1.428958
O	0.841957	-1.159248	0.860826
O	-0.441904	-1.741576	-1.316437
O	-0.210067	1.580328	0.747299
O	2.639014	1.120781	1.055115
O	-3.290994	-1.283031	-1.623255
O	-3.045341	2.006248	0.245538
O	2.392370	-2.168496	-0.814688
O	-0.951263	-3.407898	0.471626
O	0.300283	3.245648	-1.039758
O	5.741443	2.011373	0.736905
O	-6.393432	-2.172626	-1.304044
O	4.537767	-4.359280	0.245197

O	0.926815	6.293663	-0.125909
O	4.630001	2.006780	-3.383707
O	-5.281981	-2.169031	2.815567
O	-3.738849	2.818898	-4.582599
O	3.085879	-2.981146	4.013449
O	-0.236118	-4.907053	-4.185805
O	-0.416852	4.745805	3.616657
O	-4.691674	-5.286414	-4.268298
O	7.062709	-1.644725	-2.516984
O	-1.956627	6.825595	-3.701055
O	4.795346	0.293593	3.346814
O	-5.447326	-0.454843	-3.914953
O	-3.864389	4.510801	2.154828
O	3.212409	-4.673051	-2.722969
O	-3.134446	-5.167398	2.122819
O	2.482466	5.005148	-2.690959
O	4.039685	5.124162	3.701157
N	-5.383912	-4.524531	-3.577269
N	6.581833	-2.549928	-1.819221
N	-1.115014	6.936554	-2.797912
N	4.102117	1.054479	4.036832
N	-4.755088	-1.216727	-4.605982
N	-4.345256	3.605599	2.851592
N	3.692285	-3.766847	-3.420740
N	-2.291832	-5.056439	3.025971
N	1.640852	4.894189	-3.594103
N	4.730923	4.362279	3.010119
O	-6.589661	-4.336664	-3.816212
O	7.040607	-3.705050	-1.836172
O	-0.340195	7.905183	-2.738763
O	2.897360	1.243343	3.798900
O	-3.550330	-1.404591	-4.368048
O	-3.886490	2.450476	2.835640
O	3.234510	-2.612726	-3.403781
O	-1.518013	-4.086810	3.085113
O	0.865033	3.924560	-3.653263
O	5.936681	4.175414	3.248064
O	-7.246343	-1.474107	5.752648
O	2.755840	-4.714165	7.153125
O	8.320004	-0.233189	0.071665
O	-2.607085	5.922338	4.742477
O	-4.867600	-3.923558	-2.625217
O	5.613012	-2.308035	-1.086794
O	-1.030461	6.056829	-1.928793
O	4.618430	1.655451	4.988884
O	-5.271410	-1.817701	-5.557034
O	-5.314076	3.847493	3.584018
O	4.662096	-4.009743	-4.152159
O	-2.208270	-5.935162	3.894083

O	1.556291	5.773912	-4.462222
O	4.215610	3.761306	2.058076
O	-7.841260	-0.418422	3.966048
O	2.533944	-5.938650	5.387580
O	6.774918	-0.472578	1.558789
O	-4.153189	5.682946	6.231592
O	7.188280	0.256172	-4.534198
N	-7.934424	-1.434810	4.692228
N	3.283001	-5.434594	6.257621
N	7.751590	-0.955696	0.939971
N	-3.175508	5.199830	5.611784
N	7.282454	1.273561	-5.261367
O	-8.652722	-2.365936	4.365669
O	4.489345	-5.621921	6.219558
O	8.147857	-2.081320	1.191504
O	-2.778242	4.073205	5.863324
O	8.001742	2.203685	-4.933801
H	2.652112	1.105340	1.791241
H	-3.304101	-1.266593	-2.358380
H	-3.202993	2.100911	0.958278
H	2.550013	-2.263161	-1.526428
H	-1.118945	-3.517224	1.179875
H	0.466965	3.355974	-1.748013
H	4.535808	-0.476632	-1.108322
H	-5.188788	0.315382	0.540174
H	-2.085493	4.213313	-1.999272
H	1.432513	-4.375563	1.431122
H	-2.783343	-3.916049	-2.215653
H	2.131363	3.754799	1.647515
H	1.456243	0.586475	-1.663133
H	-2.108223	-0.747725	1.094995
H	-1.422893	0.977233	-2.074369
H	0.770923	-1.138482	1.505231
H	-0.312939	-1.737379	-1.952250
H	-0.340031	1.575131	1.383100
H	2.948210	3.465338	-1.331531
H	-3.601199	-3.626590	0.764383
H	-4.655390	0.856074	-2.467913
H	4.004401	-1.017326	1.900783
H	1.396521	-4.498503	-1.669596
H	-2.048501	4.335252	1.101454
O	-4.484508	5.300757	-3.355696
O	-5.188756	4.197028	-0.812328
O	-6.360550	2.996136	-3.232758
O	-2.280991	-6.663287	-3.207342
O	-1.578795	-6.455913	-0.442232
O	0.540212	-7.112840	-2.378744
O	6.594364	1.312856	-6.320787
H	-4.069211	2.020825	-5.002268

H	-3.142157	3.399631	-5.058898
H	-6.725575	2.109318	-3.264907
H	-6.899869	3.746825	-3.493361
H	-5.201891	5.532155	-3.949995
H	-3.833566	5.962060	-3.108297
H	-5.893371	3.749339	-0.339781
H	-4.863384	5.045309	-0.498613
H	-2.074258	-7.273574	-0.532471
H	-1.420821	-6.083665	0.429014
H	0.198756	-8.004548	-2.471684
H	1.488221	-6.959173	-2.369561
H	-2.480311	-7.545847	-2.886914
H	-2.733652	-6.319629	-3.979949
H	-0.487357	-5.459521	-4.929270
H	0.276558	-4.108936	-4.332454
H	-5.633172	-2.890940	3.340894
H	-4.798692	-1.457019	3.240501
H	-8.279056	-1.976915	1.215784
H	-7.632418	-0.459527	1.420808
H	-7.091393	-4.420551	0.312112
H	-6.063387	-4.709378	1.586241
H	-6.930003	-2.914884	-1.593530
H	-6.222548	-1.443511	-1.904050
H	2.082672	6.158378	3.411820
H	1.829350	7.384601	2.316784
H	-2.139201	6.796922	1.801430
H	-0.852735	7.843298	1.903527
H	-0.929537	3.947686	3.764306
H	-0.165613	5.298273	4.360122
H	0.768832	5.921412	-0.996154
H	1.422278	7.111324	-0.035670
H	5.568568	1.281261	1.335891
H	6.277014	2.752632	1.026380
H	5.408389	4.548125	-2.152408
H	6.439422	4.258303	-0.881253
H	6.980438	0.297276	-1.988948
H	7.627077	1.815665	-1.783923
H	4.146722	1.294770	-3.809642
H	4.981192	2.728690	-3.909035
H	6.246880	-3.908077	2.926213
H	6.072586	-2.270570	2.697759
H	4.213395	-5.205562	-0.068505
H	5.242373	-3.909593	-0.226347
H	3.181586	-6.124310	2.540157
H	4.550920	-5.694404	3.380864
H	2.489186	-3.561879	4.489748
H	3.417231	-2.183075	4.434127
Ga	-0.819996	-5.455746	-2.194254
Ga	4.925088	1.983536	-1.257890

Ga -4.334487 3.302187 -2.578147

XYZ of Ga<sub>11</sub>In<sub>2</sub>O

193

In	-5.445286	-2.230993	0.743041
In	-4.265169	3.302475	-2.401670
Ga	-0.217619	-0.097311	-0.203247
Ga	2.862208	-0.524312	0.142919
Ga	-3.298447	0.329682	-0.549420
Ga	-1.389025	2.800917	-0.323863
Ga	0.952781	-2.995572	-0.081637
Ga	-2.098014	-2.561169	-0.631535
Ga	1.662783	2.365548	0.225015
O	4.275067	0.106141	-0.977193
O	-4.710306	-0.300762	0.570698
O	-2.322276	3.638828	-1.764917
O	1.886037	-3.833457	1.358417
O	-2.024692	-3.877014	-2.014973
O	1.589470	3.680393	1.608428
O	3.183546	2.929825	-0.774178
O	-3.618777	-3.125446	0.367658
O	-4.254401	1.301658	-1.880155
O	3.818157	-1.496313	1.474655
O	0.897298	-4.391714	-1.378746
O	-1.333533	4.196059	0.973220
O	6.959074	1.307163	-1.689154
O	-7.395308	-1.501767	1.281654
O	4.000715	-5.512823	2.724206
O	1.692960	6.431469	2.864114
O	5.809525	4.025068	-1.318063
O	-6.245760	-4.220723	0.912537
O	5.854970	-3.189511	2.649628
O	-1.136534	6.875183	2.059508
O	1.478946	0.557613	-0.931146
O	-1.913169	-0.754226	0.524606
O	-1.398750	0.996348	-1.317987
O	0.964520	-1.191961	0.911472
O	-0.323324	-1.734697	-1.273654
O	-0.111909	1.540101	0.866159
O	2.742351	1.098729	1.151779
O	-3.177582	-1.294350	-1.558299
O	-2.952885	1.952502	0.385809
O	2.516659	-2.148106	-0.793334
O	-0.810567	-3.446703	0.477026
O	0.376337	3.251090	-0.883541
O	5.835504	2.023917	0.842070
O	-6.270748	-2.218563	-1.247565
O	4.685580	-4.343940	0.206522
O	0.979998	6.282392	0.098735

O	4.706853	2.105577	-3.273055
O	-5.142084	-2.301198	2.866535
O	-3.673745	2.871348	-4.419224
O	3.237519	-3.066952	4.011699
O	-0.101889	-4.830459	-4.216967
O	-0.334344	4.635855	3.809467
O	-4.554261	-5.247203	-4.290504
O	7.175046	-1.543477	-2.501569
O	-1.922976	6.872012	-3.451470
O	4.915445	0.237439	3.414906
O	-5.350684	-0.432061	-3.821400
O	-3.785800	4.404506	2.356327
O	3.350569	-4.600127	-2.762847
O	-2.971314	-5.263477	2.095380
O	2.536084	5.067856	-2.501900
O	4.119025	5.051557	3.884983
N	-5.250234	-4.507796	-3.579111
N	6.705045	-2.468925	-1.823222
N	-1.078581	6.969323	-2.549350
N	4.218485	0.975864	4.125268
N	-4.654711	-1.171468	-4.532793
N	-4.255795	3.479084	3.033674
N	3.819561	-3.673688	-3.441174
N	-2.125919	-5.166157	2.997506
N	1.691689	4.970544	-3.404020
N	4.813998	4.312141	3.173585
O	-6.458573	-4.325085	-3.808785
O	7.173838	-3.619232	-1.868978
O	-0.312028	7.943128	-2.470689
O	3.011133	1.159558	3.896625
O	-3.447366	-1.354162	-4.304125
O	-3.787008	2.328751	2.988917
O	3.351777	-2.524372	-3.395437
O	-1.360375	-4.191361	3.076186
O	0.924145	3.995732	-3.482712
O	6.022334	4.130455	3.402284
O	-7.100104	-1.692361	5.826865
O	2.935847	-4.875565	7.111338
O	8.430796	-0.181619	0.114299
O	-2.530045	5.766389	4.971194
O	-4.735208	-3.924642	-2.615352
O	5.737229	-2.252758	-1.081483
O	-0.982683	6.070353	-1.701358
O	4.733511	1.559018	5.089027
O	-5.169742	-1.754647	-5.495552
O	-5.223612	3.695250	3.775413
O	4.788381	-3.890871	-4.181933
O	-2.031025	-6.064110	3.844517
O	1.595786	5.869489	-4.251012



O	4.299973	3.728996	2.209832
O	-7.711734	-0.600608	4.067797
O	2.717266	-6.060462	5.318577
O	6.894122	-0.469283	1.601584
O	-4.067729	5.478667	6.460474
O	7.275504	0.404978	-4.474323
N	-7.792949	-1.634437	4.770409
N	3.465530	-5.570224	6.197154
N	7.872378	-0.929178	0.967757
N	-3.088467	5.018805	5.825652
N	7.357715	1.439841	-5.177903
O	-8.504434	-2.564015	4.425064
O	4.673297	-5.745930	6.149910
O	8.279535	-2.056812	1.191348
O	-2.680303	3.890180	6.049223
O	8.070203	2.368402	-4.831579
H	2.758675	1.066244	1.887286
H	-3.193919	-1.260891	-2.292781
H	-3.108365	2.029120	1.101189
H	2.672135	-2.224749	-1.507714
H	-0.974311	-3.573994	1.183191
H	0.539072	3.379373	-1.589686
H	4.643955	-0.430955	-1.055932
H	-5.080194	0.236325	0.649431
H	-2.021825	4.219719	-1.810659
H	1.585595	-4.415349	1.404134
H	-2.649396	-3.908243	-2.214051
H	2.214157	3.713622	1.807557
H	1.552901	0.617509	-1.573461
H	-1.988140	-0.812131	1.166966
H	-1.331247	0.992260	-1.963959
H	0.896013	-1.186856	1.556464
H	-0.197072	-1.714534	-1.909705
H	-0.239153	1.518930	1.502180
H	3.020991	3.500946	-1.180675
H	-3.457235	-3.695602	0.775175
H	-4.564184	0.851713	-2.347313
H	4.129940	-1.046351	1.941823
H	1.537661	-4.466264	-1.698442
H	-1.972883	4.269643	1.291896
O	-4.435941	5.317228	-3.131726
O	-5.119816	4.148302	-0.612037
O	-6.291206	2.993856	-3.055154
O	-2.127186	-6.627057	-3.271628
O	-1.415229	-6.478013	-0.505255
O	0.701298	-7.070829	-2.465028
O	6.664865	1.497739	-6.233360
H	-3.998868	2.080386	-4.856095
H	-3.084163	3.468286	-4.884210

H	-6.648587	2.104834	-3.106548
H	-6.838164	3.745616	-3.295999
H	-5.157810	5.556064	-3.717589
H	-3.789779	5.978315	-2.871551
H	-5.818496	3.683499	-0.147264
H	-4.800567	4.991883	-0.279897
H	-1.903890	-7.297699	-0.612587
H	-1.256862	-6.124798	0.373808
H	0.367273	-7.963113	-2.577404
H	1.647957	-6.909035	-2.456045
H	-2.317426	-7.518578	-2.971106
H	-2.586077	-6.269495	-4.034185
H	-0.351402	-5.367641	-4.972121
H	0.403161	-4.024634	-4.346981
H	-5.484733	-3.038241	3.376257
H	-4.663265	-1.595040	3.306049
H	-8.147416	-2.098357	1.283656
H	-7.513228	-0.580500	1.521478
H	-6.942214	-4.509652	0.318425
H	-5.906379	-4.819004	1.581346
H	-6.802012	-2.958588	-1.552163
H	-6.108772	-1.474172	-1.831057
H	2.151838	6.074881	3.627696
H	1.883197	7.324016	2.562617
H	-2.082187	6.713422	2.049530
H	-0.804512	7.768475	2.170899
H	-0.839400	3.830004	3.940481
H	-0.084832	5.173037	4.564622
H	0.821626	5.929152	-0.779329
H	1.468659	7.102078	0.206067
H	5.671542	1.278534	1.424526
H	6.365777	2.762934	1.146637
H	5.468130	4.624307	-1.985857
H	6.506989	4.314056	-0.725945
H	7.077998	0.384879	-1.927998
H	7.712177	1.903736	-1.690151
H	4.228040	1.399445	-3.713569
H	5.049503	2.842620	-3.782777
H	6.401920	-3.940271	2.890498
H	6.212343	-2.299489	2.701047
H	4.367314	-5.185514	-0.125562
H	5.384238	-3.877163	-0.257201
H	3.354548	-6.173937	2.465031
H	4.723584	-5.751652	3.310074
H	2.647938	-3.663890	4.476685
H	3.563637	-2.276007	4.449575
Ga	-0.672575	-5.430587	-2.236457
Ga	3.829943	-3.498071	1.994150
Ga	5.011055	2.035380	-1.149556

Ga 0.237345 5.234966 1.829937

XYZ of Ga<sub>11</sub>In<sub>2</sub>m

193

In	-5.647425	-1.870839	0.688736
In	0.489948	5.254372	1.570885
Ga	-0.281136	-0.115230	-0.258544
Ga	2.759958	-0.723903	0.152260
Ga	-3.323229	0.493499	-0.669368
Ga	-1.261591	2.844742	-0.511017
Ga	0.698300	-3.075130	-0.005091
Ga	-2.310678	-2.469107	-0.619280
Ga	1.748350	2.237649	0.102206
O	4.225075	-0.230472	-0.969458
O	-4.787348	0.000012	0.452371
O	-2.119924	3.682061	-1.998245
O	1.556653	-3.912465	1.481138
O	-2.304216	-3.841405	-1.948746
O	1.741832	3.608949	1.431687
O	3.315286	2.663052	-0.894417
O	-3.877615	-2.894510	0.377344
O	-4.197019	1.470379	-2.051988
O	3.633728	-1.700768	1.535880
O	0.569929	-4.515802	-1.247172
O	-1.133276	4.284415	0.731078
O	6.990020	0.767064	-1.685865
O	-7.553271	-0.997483	1.167757
O	3.540597	-5.667348	2.944650
O	2.005993	6.395963	2.580012
O	6.013307	3.565564	-1.439659
O	-6.576654	-3.796951	0.923564
O	5.541584	-3.472126	2.808070
O	-0.778227	6.986908	1.714440
O	1.463511	0.400216	-0.984917
O	-2.024897	-0.632728	0.467879
O	-1.374601	1.006043	-1.433655
O	0.813271	-1.237556	0.916603
O	-0.478142	-1.784152	-1.265453
O	-0.084111	1.553677	0.747366
O	2.731772	0.942657	1.094710
O	-3.294101	-1.174114	-1.611783
O	-2.886054	2.127146	0.206809
O	2.322747	-2.358563	-0.724902
O	-1.097630	-3.389889	0.543163
O	0.536300	3.158376	-1.060215
O	5.881924	1.655145	0.797415
O	-6.444217	-1.885589	-1.313502
O	4.332316	-4.646593	0.394101
O	1.321196	6.181886	-0.188216

O	4.814898	1.643542	-3.334908
O	-5.377227	-1.874999	2.817835
O	-3.483165	2.896599	-4.641248
O	2.919858	-3.128016	4.123155
O	-0.418191	-5.003356	-4.081300
O	-0.145060	4.772937	3.563192
O	-4.886821	-5.137385	-4.208118
O	7.032402	-2.121852	-2.382409
O	-1.490965	6.812833	-3.803810
O	4.814985	0.035797	3.423600
O	-5.377257	-0.266257	-3.940687
O	-3.584914	4.704457	2.066398
O	3.022586	-4.935915	-2.583471
O	-3.392018	-4.998479	2.197486
O	2.829690	4.767022	-2.714559
O	4.324472	4.905943	3.692045
N	-5.542941	-4.327068	-3.537243
N	6.494873	-2.987409	-1.675739
N	-0.653946	6.892119	-2.893093
N	4.157830	0.845156	4.093469
N	-4.721137	-1.076574	-4.611562
N	-4.122423	3.838886	2.772068
N	3.559172	-4.069305	-3.290175
N	-2.554000	-4.919249	3.108224
N	1.992670	4.687736	-3.625276
N	4.979594	4.095681	3.021149
O	-6.733875	-4.076890	-3.792788
O	6.889095	-4.166227	-1.669017
O	0.172692	7.817327	-2.840684
O	2.967930	1.096293	3.838930
O	-3.531181	-1.326712	-4.357038
O	-3.728221	2.660083	2.779790
O	3.165893	-2.891541	-3.296863
O	-1.728305	-3.992987	3.160597
O	1.164979	3.761585	-3.677691
O	6.170604	3.846486	3.275680
O	-7.330543	-1.023990	5.721010
O	2.461637	-4.787806	7.286219
O	8.338951	-0.739133	0.197386
O	-2.278346	6.087162	4.645193
O	-5.004065	-3.739807	-2.589146
O	5.533369	-2.680255	-0.958285
O	-0.627318	6.023615	-2.009110
O	4.696706	1.432418	5.041565
O	-5.260033	-1.663820	-5.558659
O	-5.083927	4.146040	3.489523
O	4.521598	-4.377498	-4.006596
O	-2.528295	-5.786714	3.991172
O	1.966023	5.556255	-4.508259

O	4.441717	3.508365	2.073073
O	-7.847422	0.033137	3.911132
O	2.190634	-6.027306	5.538092
O	6.767575	-0.868106	1.670573
O	-3.850759	5.958275	6.120358
O	7.284096	-0.264539	-4.428226
N	-8.004312	-0.964360	4.652380
N	2.957368	-5.551016	6.408377
N	7.722370	-1.414631	1.070653
N	-2.894946	5.411679	5.519460
N	7.442059	0.733886	-5.170467
O	-8.769656	-1.859688	4.332653
O	4.151811	-5.805286	6.386967
O	8.053022	-2.556092	1.344629
O	-2.563351	4.269164	5.793470
O	8.208326	1.628175	-4.849705
H	2.736329	0.938738	1.831090
H	-3.298622	-1.169182	-2.347177
H	-3.045631	2.242188	0.916114
H	2.482305	-2.473590	-1.433207
H	-1.278477	-3.478016	1.251127
H	0.716204	3.247556	-1.768214
H	4.559571	-0.792765	-1.021295
H	-5.122842	0.562361	0.504188
H	-1.782078	4.240264	-2.062020
H	1.218751	-4.471666	1.544926
H	-2.926971	-3.840620	-2.156200
H	2.364698	3.610161	1.639113
H	1.549582	0.429440	-1.627851
H	-2.111854	-0.659899	1.110764
H	-1.299045	0.971729	-2.077834
H	0.736792	-1.202204	1.559747
H	-0.342530	-1.797638	-1.899751
H	-0.220777	1.566220	1.381658
H	3.195226	3.226619	-1.325489
H	-3.758517	-3.457008	0.809380
H	-4.529016	1.022762	-2.505937
H	3.967722	-1.253262	1.989870
H	1.208289	-4.643884	-1.553638
H	-1.770673	4.411428	1.036579
O	-4.102905	5.435875	-3.462723
O	-4.893666	4.415095	-0.910154
O	-6.104931	3.240739	-3.324165
O	-2.567303	-6.627491	-3.098064
O	-1.883525	-6.413344	-0.328857
O	0.215878	-7.218351	-2.230513
O	6.768271	0.793531	-6.238097
H	-3.852849	2.111133	-5.051807
H	-2.850287	3.435504	-5.119996

H	-6.518175	2.375022	-3.346250
H	-6.599087	4.015638	-3.602830
H	-4.800138	5.696642	-4.068726
H	-3.418935	6.064234	-3.218587
H	-5.626885	4.014909	-0.438507
H	-4.525079	5.249203	-0.606388
H	-2.422562	-7.203779	-0.411604
H	-1.714249	-6.035977	0.538053
H	-0.173472	-8.091259	-2.313033
H	1.170798	-7.117143	-2.213065
H	-2.818541	-7.492256	-2.765833
H	-2.992159	-6.272231	-3.881142
H	-0.691899	-5.553370	-4.818625
H	0.139416	-4.237315	-4.234888
H	-5.773326	-2.567592	3.350637
H	-4.859682	-1.183809	3.236765
H	-8.342235	-1.544237	1.181377
H	-7.614689	-0.061683	1.369402
H	-7.282441	-4.064399	0.330409
H	-6.285338	-4.388370	1.620545
H	-7.018045	-2.601784	-1.597129
H	-6.226960	-1.177085	-1.923124
H	2.430885	6.041716	3.364076
H	2.257306	7.261711	2.246767
H	-1.732129	6.885630	1.696012
H	-0.390797	7.860910	1.795905
H	-0.702687	4.006911	3.717780
H	0.128648	5.322951	4.300518
H	1.151901	5.804534	-1.054126
H	1.860234	6.972321	-0.105470
H	5.662635	0.945738	1.406010
H	6.454699	2.370397	1.081035
H	5.720031	4.158107	-2.135695
H	6.720132	3.832926	-0.848482
H	7.052360	-0.169774	-1.886475
H	7.779962	1.313778	-1.698464
H	4.297373	0.952336	-3.754838
H	5.210997	2.336134	-3.867710
H	6.035796	-4.246026	3.086721
H	5.954884	-2.605411	2.830142
H	3.964839	-5.478759	0.090328
H	5.065627	-4.244395	-0.076574
H	2.856607	-6.295691	2.701514
H	4.238828	-5.928170	3.550674
H	2.286980	-3.666922	4.601903
H	3.290520	-2.342590	4.534734
Ga	-1.052276	-5.485830	-2.087959
Ga	3.509640	-3.676725	2.133580
Ga	5.086094	1.639326	-1.205788

Ga -4.071949 3.445252 -2.651652



XYZ of Ga<sub>11</sub>In<sub>2</sub>P

193

In	5.071626	1.605111	-1.081065
In	-5.752993	-1.715366	0.628023
Ga	-0.341143	-0.054590	-0.226530
Ga	2.681976	-0.738913	0.197679
Ga	-3.365259	0.629809	-0.650768
Ga	-1.255183	2.931202	-0.416373
Ga	0.571871	-3.040314	-0.035717
Ga	-2.417201	-2.354456	-0.663008
Ga	1.734837	2.244278	0.209937
O	4.168311	-0.250662	-0.898091
O	-4.850598	0.141481	0.445031
O	-2.080662	3.822440	-1.890810
O	1.397379	-3.931544	1.437721
O	-2.427198	-3.694262	-2.025192
O	1.744757	3.583087	1.572110
O	3.320272	2.659319	-0.761481
O	-4.002636	-2.769497	0.308409
O	-4.204216	1.658360	-2.017397
O	3.520904	-1.767472	1.565307
O	0.424749	-4.447624	-1.313455
O	-1.108138	4.337515	0.861354
O	6.960973	0.703443	-1.564393
O	-7.644227	-0.812538	1.110305
O	3.328653	-5.763763	2.876703
O	2.057509	6.335332	2.789982
O	6.042304	3.515796	-1.259598
O	-6.725694	-3.625905	0.807498
O	5.377635	-3.609911	2.811925
O	-0.704722	7.007268	1.913117
O	1.421236	0.440096	-0.923956
O	-2.102680	-0.551349	0.470902
O	-1.398647	1.118071	-1.384268
O	0.717279	-1.228327	0.931225
O	-0.564099	-1.694184	-1.275339
O	-0.118158	1.585012	0.821279
O	2.680386	0.904763	1.179898
O	-3.362749	-1.014941	-1.632969
O	-2.901675	2.232064	0.268732
O	2.218344	-2.342156	-0.722831
O	-1.235712	-3.329028	0.488031
O	0.554345	3.218772	-0.941073
O	5.847901	1.555536	0.929248
O	-6.530216	-1.664725	-1.381309
O	4.167153	-4.699530	0.359087
O	1.395485	6.202703	0.011134

O	4.821506	1.666327	-3.211889
O	-5.503869	-1.776505	2.758817
O	-3.434459	3.130468	-4.564618
O	2.751128	-3.240560	4.110518
O	-0.545748	-4.845411	-4.167622
O	-0.137505	4.736316	3.713533
O	-5.014766	-4.879187	-4.339198
O	6.948051	-2.168160	-2.330253
O	-1.366813	6.981239	-3.614119
O	4.720640	-0.102809	3.505421
O	-5.402927	-0.006372	-3.958482
O	-3.563171	4.778577	2.183596
O	2.880808	-4.888755	-2.636667
O	-3.580301	-4.926610	2.081515
O	2.897938	4.816432	-2.534586
O	4.332373	4.769001	3.887126
N	-5.659863	-4.071137	-3.655031
N	6.385117	-3.038541	-1.649776
N	-0.537266	7.020427	-2.694005
N	4.074498	0.704331	4.188549
N	-4.757829	-0.814423	-4.642649
N	-4.126076	3.908205	2.863074
N	3.442823	-4.017300	-3.317163
N	-2.749758	-4.887500	3.001658
N	2.068391	4.777244	-3.454701
N	4.976474	3.961028	3.202930
O	-6.842574	-3.789067	-3.915508
O	6.753809	-4.225471	-1.667930
O	0.308525	7.925922	-2.611527
O	2.892832	0.987311	3.929111
O	-3.576085	-1.096406	-4.383200
O	-3.757413	2.721266	2.845919
O	3.075050	-2.831444	-3.298990
O	-1.904886	-3.980930	3.084118
O	1.221526	3.870830	-3.537218
O	6.159291	3.679964	3.462418
O	-7.466848	-0.953170	5.663455
O	2.226273	-4.965445	7.228072
O	8.258638	-0.876493	0.294301
O	-2.252555	6.070252	4.807150
O	-5.117819	-3.518656	-2.688024
O	5.423442	-2.727868	-0.934067
O	-0.538006	6.130581	-1.831099
O	4.616543	1.256812	5.155556
O	-5.299903	-1.366912	-5.608656
O	-5.087751	4.218877	3.578782
O	4.405387	-4.329055	-4.031854
O	-2.751388	-5.776263	3.863546
O	2.069102	5.667082	-4.316606

O	4.435426	3.408469	2.235952
O	-7.943072	0.158083	3.874974
O	1.945855	-6.156441	5.448004
O	6.670460	-1.006603	1.749257
O	-3.841788	5.940203	6.264077
O	7.259712	-0.268183	-4.328074
N	-8.128651	-0.853273	4.590363
N	2.714073	-5.717958	6.336657
N	7.619125	-1.559196	1.145186
N	-2.892097	5.387541	5.659035
N	7.446394	0.744101	-5.044423
O	-8.909898	-1.723819	4.241949
O	3.902923	-5.997546	6.320206
O	7.922445	-2.713823	1.394508
O	-2.587859	4.231840	5.908376
O	8.228531	1.613564	-4.694992
H	2.677625	0.883071	1.915978
H	-3.359941	-0.992260	-2.368039
H	-3.065699	2.333488	0.979099
H	2.382339	-2.443589	-1.432199
H	-1.425356	-3.430171	1.191941
H	0.743069	3.320990	-1.645002
H	4.491130	-0.818688	-0.960414
H	-5.174413	0.709585	0.507325
H	-1.730278	4.374537	-1.937906
H	1.046918	-4.484638	1.484806
H	-3.047725	-3.674960	-2.238349
H	2.365439	3.565779	1.785288
H	1.514225	0.482866	-1.565165
H	-2.196511	-0.592047	1.112105
H	-1.317522	1.097597	-2.028358
H	0.635265	-1.206769	1.574298
H	-0.422586	-1.695386	-1.908490
H	-0.260745	1.585294	1.454390
H	3.216600	3.235548	-1.179879
H	-3.899912	-3.344659	0.727789
H	-4.541289	1.229092	-2.485118
H	3.859970	-1.338358	2.033085
H	1.063185	-4.582159	-1.616982
H	-1.745626	4.470984	1.163900
O	-4.010987	5.653594	-3.330774
O	-4.848549	4.589266	-0.811131
O	-6.061025	3.499803	-3.264026
O	-2.738847	-6.445579	-3.244024
O	-2.077849	-6.312881	-0.464205
O	0.022329	-7.117454	-2.365189
O	6.784562	0.843989	-6.116515
H	-3.816901	2.363305	-4.997493
H	-2.785466	3.666825	-5.024272

H	-6.492556	2.644054	-3.310906
H	-6.535640	4.291726	-3.528431
H	-4.696465	5.943927	-3.936743
H	-3.316091	6.260895	-3.065146
H	-5.594802	4.193907	-0.356150
H	-4.465109	5.407632	-0.483845
H	-2.632923	-7.089198	-0.571074
H	-1.909018	-5.960201	0.413123
H	-0.384876	-7.979460	-2.472436
H	0.978988	-7.037476	-2.336416
H	-3.011875	-7.312404	-2.935178
H	-3.148253	-6.062472	-4.022189
H	-0.823968	-5.371488	-4.920561
H	0.029687	-4.088206	-4.297426
H	-5.919986	-2.472914	3.270988
H	-4.975718	-1.106984	3.199154
H	-8.444864	-1.342182	1.103345
H	-7.687481	0.119266	1.333967
H	-7.431211	-3.863632	0.201504
H	-6.454024	-4.240077	1.492634
H	-7.116502	-2.361263	-1.687516
H	-6.291795	-0.946682	-1.971552
H	2.466963	5.953214	3.569157
H	2.330644	7.203162	2.480147
H	-1.660355	6.927221	1.883373
H	-0.299403	7.870434	2.019318
H	-0.712970	3.979103	3.844337
H	0.140714	5.262393	4.466472
H	1.226625	5.850015	-0.865195
H	1.950560	6.979020	0.118003
H	5.607439	0.836659	1.518423
H	6.433113	2.251154	1.235416
H	5.768690	4.131112	-1.943782
H	6.748876	3.753463	-0.655575
H	7.005118	-0.229444	-1.787038
H	7.762577	1.233001	-1.556406
H	4.293383	0.996815	-3.653225
H	5.237622	2.362736	-3.724060
H	5.852328	-4.400838	3.076341
H	5.809243	-2.753166	2.858817
H	3.784863	-5.515980	0.031852
H	4.913531	-4.302186	-0.094872
H	2.633727	-6.371072	2.612074
H	4.015127	-6.054174	3.482701
H	2.102135	-3.776917	4.570172
H	3.134537	-2.473483	4.544422
Ga	-1.209609	-5.361697	-2.192529
Ga	3.348483	-3.754042	2.113812
Ga	0.527245	5.251519	1.739458

Ga -4.030817 3.643873 -2.567883

XYZ of Ga<sub>12</sub>In<sub>1</sub>

193

In	-5.623284	-1.870232	0.667283
Ga	-0.273861	-0.042794	-0.238644
Ga	2.772749	-0.629080	0.163765
Ga	-3.321471	0.543538	-0.641074
Ga	-1.283614	2.911653	-0.433849
Ga	0.734872	-2.997200	-0.042460
Ga	-2.279390	-2.409227	-0.648227
Ga	1.731621	2.322640	0.170933
O	4.233999	-0.099000	-0.946217
O	-4.781722	0.013412	0.468928
O	-2.148764	3.769566	-1.905307
O	1.600043	-3.855109	1.427998
O	-2.257849	-3.754875	-2.004506
O	1.710035	3.667289	1.527207
O	3.295239	2.783255	-0.815196
O	-3.843008	-2.869842	0.337903
O	-4.203579	1.538758	-2.005208
O	3.654836	-1.624305	1.528899
O	0.622182	-4.414276	-1.312884
O	-1.170970	4.327730	0.836569
O	6.989556	0.940030	-1.639437
O	-7.538257	-1.025568	1.161129
O	3.599948	-5.618659	2.859006
O	1.945138	6.433583	2.730625
O	5.984652	3.723236	-1.339242
O	-6.533440	-3.809782	0.862927
O	5.579017	-3.401308	2.768205
O	-0.843970	7.013689	1.873500
O	1.466282	0.504279	-0.952583
O	-2.013098	-0.591911	0.475304
O	-1.377289	1.090494	-1.392728
O	0.830520	-1.177127	0.915455
O	-0.453139	-1.693392	-1.278530
O	-0.094563	1.607809	0.800242
O	2.726936	1.018182	1.138883
O	-3.274705	-1.104769	-1.616177
O	-2.901549	2.163848	0.267701
O	2.352803	-2.250384	-0.746016
O	-1.058378	-3.340630	0.497292
O	0.511608	3.253997	-0.974565
O	5.870106	1.767804	0.859535
O	-6.417850	-1.853397	-1.335823
O	4.384015	-4.539893	0.330061
O	1.265336	6.267383	-0.042118
O	4.807457	1.827146	-3.273506

O	-5.355226	-1.913733	2.796212
O	-3.501389	3.022877	-4.564950
O	2.952643	-3.109414	4.086636
O	-0.358127	-4.855613	-4.157280
O	-0.190574	4.770075	3.678971
O	-4.825061	-5.031701	-4.292150
O	7.061540	-1.934003	-2.392803
O	-1.549313	6.941500	-3.647972
O	4.816742	0.086351	3.451954
O	-5.364465	-0.171939	-3.929242
O	-3.628046	4.696837	2.176937
O	3.080277	-4.783424	-2.654230
O	-3.338246	-5.004388	2.116760
O	2.790477	4.917801	-2.594054
O	4.277271	4.945109	3.815856
N	-5.489935	-4.241377	-3.606213
N	6.531976	-2.818665	-1.704005
N	-0.714056	7.011137	-2.734851
N	4.150844	0.875727	4.136865
N	-4.699590	-0.962264	-4.615179
N	-4.157589	3.812179	2.864735
N	3.608888	-3.897717	-3.343043
N	-2.501990	-4.934796	3.029902
N	1.955220	4.848163	-3.507175
N	4.941147	4.154831	3.129898
O	-6.683052	-3.998099	-3.858218
O	6.937961	-3.993393	-1.720067
O	0.103233	7.943334	-2.663191
O	2.958751	1.119953	3.885886
O	-3.507452	-1.205491	-4.364194
O	-3.751624	2.637447	2.849672
O	3.203855	-2.724034	-3.326966
O	-1.685654	-4.001555	3.101547
O	1.136887	3.915014	-3.578862
O	6.134330	3.912557	3.380910
O	-7.319912	-1.139749	5.713238
O	2.507825	-4.835824	7.215771
O	8.351566	-0.589520	0.215362
O	-2.337999	6.041325	4.784102
O	-4.957926	-3.667601	-2.646058
O	5.566718	-2.535347	-0.981798
O	-0.679643	6.125658	-1.868148
O	4.682853	1.449503	5.097020
O	-5.231621	-1.536044	-5.574335
O	-5.122846	4.095497	3.586942
O	4.575078	-4.182084	-4.064236
O	-2.468509	-5.819226	3.895590
O	1.920786	5.733638	-4.372878
O	4.410136	3.581009	2.169764

O	-7.845495	-0.052303	3.923948
O	2.251012	-6.043208	5.443197
O	6.780060	-0.763231	1.683806
O	-3.910545	5.867650	6.254524
O	7.296727	-0.034238	-4.401262
N	-7.993154	-1.065757	4.645175
N	3.012058	-5.576567	6.323642
N	7.740883	-1.288249	1.074379
N	-2.948702	5.342591	5.644119
N	7.445453	0.980174	-5.123463
O	-8.749180	-1.962191	4.306913
O	4.209006	-5.818432	6.298671
O	8.082657	-2.431540	1.326178
O	-2.605976	4.198255	5.895933
O	8.202410	1.875558	-4.784186
H	2.730782	0.999770	1.875047
H	-3.278526	-1.085363	-2.351336
H	-3.062991	2.263264	0.978944
H	2.514224	-2.349806	-1.456258
H	-1.239055	-3.444518	1.203159
H	0.691332	3.358930	-1.680447
H	4.574155	-0.656794	-1.008733
H	-5.122876	0.571252	0.531424
H	-1.816453	4.332264	-1.957643
H	1.267686	-4.418805	1.480328
H	-2.880369	-3.756209	-2.212661
H	2.332647	3.670621	1.735373
H	1.552711	0.547049	-1.594710
H	-2.100434	-0.632637	1.117422
H	-1.300737	1.069662	-2.037367
H	0.753035	-1.155245	1.559079
H	-0.316754	-1.692998	-1.912806
H	-0.231993	1.606461	1.434491
H	3.169987	3.353996	-1.235208
H	-3.718730	-3.439543	0.758899
H	-4.530620	1.096900	-2.468305
H	3.983875	-1.182539	1.992037
H	1.262102	-4.529905	-1.621041
H	-1.809916	4.442319	1.143742
O	-4.147696	5.532077	-3.337299
O	-4.930806	4.453255	-0.806334
O	-6.127806	3.314763	-3.244519
O	-2.491887	-6.520212	-3.208898
O	-1.813105	-6.353970	-0.435176
O	0.296180	-7.100281	-2.349794
O	6.772189	1.054161	-6.190527
H	-3.862780	2.242020	-4.991378
H	-2.873446	3.577420	-5.032201
H	-6.532348	2.445570	-3.284186



H	-6.629403	4.090042	-3.508439
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H	-3.470293	6.162287	-3.079980
H	-5.660466	4.036538	-0.343568
H	-4.570890	5.284840	-0.485720
H	-2.344125	-7.147957	-0.534160
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H	-0.625568	-5.393665	-4.905648
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H	-5.744920	-2.620629	3.314761
H	-4.845047	-1.225819	3.229329
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H	-6.236934	-4.411912	1.548455
H	-6.984197	-2.569543	-1.634226
H	-6.207070	-1.130861	-1.931081
H	2.372753	6.068182	3.508062
H	2.188119	7.308208	2.414836
H	-1.796792	6.903279	1.851918
H	-0.465384	7.889735	1.972667
H	-0.740669	3.995619	3.817735
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H	1.796356	7.061370	0.056866
H	5.657303	1.044365	1.453745
H	6.435408	2.482997	1.157911
H	5.686173	4.326451	-2.023806
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H	4.300136	-5.884415	3.460613
H	2.324699	-3.663956	4.553886
H	3.315012	-2.328607	4.514084
Ga	-0.989384	-5.383655	-2.174620
Ga	3.549909	-3.612818	2.087338
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Ga 5.076514 1.783599 -1.144556

XYZ of Ga<sub>13</sub>

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Ga	-0.348120	-0.085005	-0.227292
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O	1.708307	-3.801611	1.440313
O	-2.169727	-3.890218	-1.969741
O	1.473486	3.718208	1.515153
O	3.084146	2.899826	-0.833734
O	-3.780387	-3.070836	0.379148
O	-4.356346	1.308540	-1.975691
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O	6.854386	1.225226	-1.673872
O	-7.551612	-1.395234	1.218274
O	3.795216	-5.466647	2.865088
O	1.588267	6.496475	2.708439
O	5.724534	3.960408	-1.376549
O	-6.421790	-4.131420	0.922949
O	5.669874	-3.161157	2.755657
O	-1.229394	6.945073	1.865908
O	1.360960	0.538883	-0.953174
O	-2.056200	-0.710893	0.498602
O	-1.508997	0.992512	-1.378434
O	0.813756	-1.163522	0.923863
O	-0.457406	-1.745637	-1.260895
O	-0.238819	1.575629	0.805312
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O	2.374149	-2.171484	-0.743139
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O	-6.408717	-2.179322	-1.282602
O	4.514438	-4.361699	0.328186
O	0.900931	6.289779	-0.059720
O	4.624542	2.005702	-3.297868
O	-5.320783	-2.176712	2.843282

O	-3.737694	2.814550	-4.544186
O	3.040469	-2.985557	4.088585
O	-0.233853	-4.909994	-4.130169
O	-0.463373	4.739987	3.674570
O	-4.688696	-5.291295	-4.238208
O	7.053888	-1.645038	-2.418582
O	-1.962309	6.821718	-3.651065
O	4.752256	0.290176	3.432877
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O	-3.902412	4.503982	2.193018
O	3.206171	-4.674992	-2.647603
O	-3.168000	-5.173881	2.161728
O	2.471759	5.002871	-2.616313
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N	-4.386842	3.598319	2.886705
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O	2.851300	1.238925	3.874467
O	-3.548526	-1.408932	-4.330066
O	-3.927481	2.443404	2.872959
O	3.231240	-2.614414	-3.327544
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O	0.860321	3.921913	-3.588212
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O	-7.302174	-1.483709	5.769358
O	2.693297	-4.719847	7.225711
O	8.295770	-0.233874	0.177698
O	-2.660514	5.915148	4.788298
O	-4.874596	-3.929106	-2.595673
O	5.596352	-2.309501	-0.996921
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O	4.565372	1.651367	5.074395
O	-5.262613	-1.822377	-5.528996
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O	1.555360	5.771861	-4.392556
O	4.178340	3.758094	2.142087
O	-7.887359	-0.427647	3.979770

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H	1.402478	-4.379779	1.496374
H	-2.792713	-3.920822	-2.174225
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H	0.739039	-1.143018	1.567859
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H	3.970154	-1.020574	1.981892
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H	-2.080467	4.329614	1.149955
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O	-6.367130	2.990144	-3.209257
O	-2.283493	-6.667482	-3.164010
O	-1.597172	-6.460789	-0.394866
O	0.533138	-7.116085	-2.319494
O	6.605933	1.313699	-6.223942
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H	-3.138553	3.395716	-5.016867
H	-6.731572	2.103177	-3.243803
H	-6.905287	3.740688	-3.472666

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H	1.481011	-6.962002	-2.304849
H	-2.484245	-7.550246	-2.845038
H	-2.731892	-6.323747	-3.939064
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H	5.394765	4.546949	-2.061245
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H	4.978402	2.727955	-3.820927
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H	6.034316	-2.273189	2.790205
H	4.192237	-5.208012	0.012337
H	5.221523	-3.911532	-0.139171
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H	4.510299	-5.697940	3.463401
H	2.441327	-3.566724	4.561267
H	3.369062	-2.187491	4.511430
Ga	-0.828836	-5.459658	-2.142175
Ga	3.648744	-3.467864	2.087407
Ga	0.132596	5.288648	1.687590
Ga	-4.344970	3.296857	-2.542992
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