

Cluster formula	6-311++ . conv.	Enthalpy (hartree)	Entropy (cal K <sup>-1</sup> mol <sup>-1</sup> )	Gibbs free energy (hartree)
S <sub>4</sub>	56	-2801.256008	179.461	-2801.341276
S <sub>4</sub> A <sub>1</sub>	169	-2857.820795	187.395	-2857.909833
S <sub>4</sub> A <sub>2</sub>	84	-2914.388489	193.997	-2914.480663
S <sub>4</sub> A <sub>3</sub>	68	-2970.94645	209.77	-2971.046119
S <sub>4</sub> A <sub>4</sub>	38	-3027.500303	225.959	-3027.607663
S <sub>4</sub> A <sub>5</sub>	34	-3084.050337	237.758	-3084.163303
S <sup>-</sup> S <sub>3</sub>	97	-2800.835072	168.993	-2800.915366
S <sup>-</sup> S <sub>3</sub> A <sub>1</sub>	122	-2857.389946	184.899	-2857.477797
S <sup>-</sup> S <sub>3</sub> A <sub>2</sub>	21	-2913.941409	192.489	-2914.032867
S <sup>-</sup> S <sub>3</sub> A <sub>3</sub>	13	-2970.490814	195.627	-2970.583762
S <sup>-</sup> S <sub>4</sub>	138	-3501.162655	200.525	-3501.257931
S <sup>-</sup> S <sub>4</sub> A <sub>1</sub>	71	-3557.727072	208.015	-3557.825907
S <sup>-</sup> S <sub>4</sub> A <sub>2</sub>	22	-3614.287482	213.397	-3614.388874
S <sup>-</sup> S <sub>4</sub> A <sub>3</sub>	23	-3670.836831	226.504	-3670.94445
S <sup>-</sup> S <sub>4</sub> A <sub>4</sub>	18	-3727.385956	237.152	-3727.498634
H <sup>+</sup> A <sub>2</sub>	16	-113.413269	68.478	-113.445805
H <sup>+</sup> A <sub>2</sub> W <sub>1</sub>	42	-189.845603	94.248	-189.890384
H <sup>+</sup> A <sub>2</sub> W <sub>2</sub>	56	-266.276653	113.49	-266.330576
H <sup>+</sup> A <sub>2</sub> W <sub>3</sub>	63	-342.706301	132.722	-342.769362
H <sup>+</sup> A <sub>2</sub> W <sub>4</sub>	114	-419.133157	160.449	-419.209391
H <sup>+</sup> A <sub>2</sub> W <sub>5</sub>	116	-495.567408	161.447	-495.644117
H <sup>+</sup> A <sub>2</sub> W <sub>6</sub>	70	-571.994961	175.085	-572.078149
H <sup>+</sup> A <sub>2</sub> W <sub>0</sub> S <sub>1</sub>	40	-813.745253	107.764	-813.796455
H <sup>+</sup> A <sub>2</sub> W <sub>1</sub> S <sub>1</sub>	173	-890.181285	121.33	-890.238933
H <sup>+</sup> A <sub>2</sub> W <sub>2</sub> S <sub>1</sub>	103	-966.618165	130.584	-966.680209
H <sup>+</sup> A <sub>2</sub> W <sub>3</sub> S <sub>1</sub>	169	-1043.047622	154.145	-1043.120861
H <sup>+</sup> A <sub>2</sub> W <sub>4</sub> S <sub>1</sub>	188	-1119.476882	177.051	-1119.561004
H <sup>+</sup> A <sub>2</sub> W <sub>5</sub> S <sub>1</sub>	178	-1195.90253	200.029	-1195.99757
H <sup>+</sup> A <sub>2</sub> W <sub>6</sub> S <sub>1</sub>	85	-1272.330781	215.117	-1272.43299