Table S1. Topological properties of the electron density at the bond critical points of the $BaRh_2Ge_4X_6$ (X = S, Se, Te) and $BaRh_2Ge_4S_4Te_2$ compounds. ρ in e/bohr^3, Δρ in e/bohr^5, G and V in Ry/ bohr^3, H/ρ and G/ρ in Ry/e, R, R_1 and R_2 in Bohr, θ in degree.

Bond	ρ(r)	Δρ(r)	G	V	|V|/G	H/ρ	G/ρ	R	R_1	R_2	R_1/R_2	θ
						$BaRh_2Ge_4S_6$						
	0.1007	0.0552	0.0718	−0.1298	1.8076	−0.5757	0.7129	2.241	0.828	1.075	0.770	176.5
	0.0862	0.0257	0.0526	−0.0988	1.8777	−0.5355	0.6101	2.331	1.046	1.285	0.814	179.5
Ge-S	0.0762	0.0468	0.0471	−0.0826	1.7515	−0.4648	0.6185	2.388	0.892	1.161	0.769	178.7
	0.0729	0.0541	0.0455	−0.0775	1.7028	−0.4391	0.6247	2.406	1.074	1.332	0.807	179.5
	0.0668	0.0384	0.0380	−0.0664	1.7474	−0.4249	0.5685	2.467	0.917	1.359	0.675	179.1
	0.0834	0.0221	0.0494	−0.0933	1.8882	−0.5261	0.5923	2.416	1.264	0.956	1.322	175.3
Rh-Ge	0.0805	0.0861	0.0575	−0.0934	1.6254	−0.4463	0.7136	2.415	1.232	1.012	1.217	176.7
	0.0804	0.0062	0.0440	−0.0865	1.9650	−0.5285	0.5476	2.438	1.268	0.978	1.296	175.8
	0.0762	0.1365	0.0621	−0.0900	1.4501	−0.3667	0.8147	2.437	1.183	1.254	0.944	179.9
Rh-S	0.0677	0.1476	0.0569	−0.0769	1.3515	−0.2954	0.8404	2.491	1.200	1.159	1.035	176.6
	0.0669	0.1502	0.0567	−0.0758	1.3375	−0.2860	0.8474	2.498	1.070	1.294	0.827	177.7
	0.0185	0.0406	0.0105	−0.0108	1.0306	−0.0173	0.5671	3.310	1.523	1.673	0.910	178.5
	0.0165	0.0374	0.0093	−0.0093	0.9965	0.0020	0.5629	3.341	1.517	1.682	0.902	177.8
Ba-S	0.0164	0.0334	0.0086	−0.0089	1.0316	−0.0165	0.5240	3.375	1.523	1.711	0.890	179.2
	0.0160	0.0307	0.0080	−0.0084	1.0465	−0.0233	0.5014	3.357	1.526	1.691	0.902	178.2
	0.0157	0.0449	0.0103	−0.0094	0.9124	0.0575	0.6557	3.328	1.397	1.671	0.836	179.3
	0.0233	0.0540	0.0144	−0.0154	1.0661	−0.0410	0.6203	2.975	1.487	1.488	1.000	180.0
	0.0097	0.0220	0.0049	−0.0044	0.8854	0.0582	0.5082	3.591	1.823	1.769	1.031	176.7
S-S	0.0081	0.0192	0.0041	−0.0035	0.8402	0.0816	0.5108	3.693	1.872	1.826	1.026	174.1
	0.0051	0.0090	0.0019	−0.0016	0.8360	0.0623	0.3800	4.266	2.152	2.143	1.004	166.7
	0.0050	0.0082	0.0018	−0.0015	0.8568	0.0508	0.3548	4.211	2.131	2.112	1.009	166.0
						$BaRh_2Ge_4Se_6$						
	0.0810	0.0120	0.0456	−0.0881	1.9342	−0.5253	0.5623	2.4200	1.0000	1.3117	0.7624	175.9
	0.0720	0.0172	0.0386	−0.0730	1.8889	−0.4769	0.5366	2.4929	1.1214	1.3715	0.8176	179.4
Ge-Se	0.0679	0.0013	0.0327	−0.0651	1.9903	−0.4765	0.4812	2.5187	1.1350	1.3842	0.8199	177.8
	0.0635	0.0198	0.0323	−0.0597	1.8470	−0.4310	0.5088	2.5489	1.1413	1.4077	0.8107	179.5
	0.0610	0.0074	0.0283	−0.0548	1.9349	−0.4346	0.4649	2.5889	1.1735	1.4157	0.8289	178.2
	0.0814	0.0745	0.0563	−0.0940	1.6692	−0.4629	0.6917	2.4268	1.2615	1.1654	1.0825	178.9
Rh-Ge	0.0795	−0.0423	0.0351	−0.0809	2.3012	−0.5753	0.4421	2.4409	1.1386	1.1776	0.9669	177.6
	0.0792	0.0630	0.0524	−0.0891	1.6995	−0.4631	0.6620	2.4220	1.2355	1.1866	1.0412	179.8
	0.0663	0.1315	0.0531	−0.0733	1.3806	−0.3048	0.8008	2.5622	1.2216	1.3406	0.9112	179.2
Rh-Se	0.0609	0.1609	0.0538	−0.0675	1.2530	−0.2239	0.8849	2.6009	1.2381	1.3629	0.9083	178.9
	0.0608	0.1591	0.0535	−0.0672	1.2565	−0.2258	0.8802	2.6017	1.2353	1.3665	0.9040	178.7
	0.0172	0.0366	0.0094	−0.0096	1.0246	−0.0134	0.5464	3.4298	1.5744	1.7660	0.8915	179.3
	0.0163	0.0343	0.0087	−0.0089	1.0181	−0.0097	0.5347	3.4275	1.5807	1.7574	0.8994	177.9
Ba-Se	0.0154	0.0289	0.0076	−0.0079	1.0444	−0.0218	0.4902	3.4561	1.5966	1.7709	0.9016	177.7
	0.0148	0.0384	0.0090	−0.0083	0.9287	0.0432	0.6057	3.5143	1.6058	1.8181	0.8832	179.0
	0.0147	0.0297	0.0075	−0.0076	1.0084	−0.0043	0.5088	3.4388	1.5762	1.5759	1.0002	179.4
	0.0234	0.0523	0.0142	−0.0154	1.0802	−0.0487	0.6076	3.0850	1.4399	1.4399	1.0000	180.0
	0.0111	0.0282	0.0063	−0.0055	0.8769	0.0699	0.5672	3.6321	1.8428	1.7917	1.0285	175.9
Se-Se	0.0090	0.0212	0.0047	−0.0040	0.8630	0.0706	0.5151	3.7587	1.9079	1.8608	1.0253	171.6
	0.0056	0.0081	0.0019	−0.0017	0.9066	0.0311	0.3331	4.3071	2.1699	2.1580	1.0055	168.7
	0.0050	0.0066	0.0015	−0.0014	0.9180	0.0249	0.3030	4.4449	2.2626	2.2554	1.0032	159.4
						$BaRh_2Ge_4Te_6$						
	0.0601	−0.0101	0.0248	−0.0521	2.1018	−0.4544	0.4125	2.7082	1.3140	1.2609	1.0421	179.4
	0.0590	−0.0090	0.0242	−0.0506	2.0929	−0.4478	0.4097	2.7282	1.5027	1.2256	1.2261	179.1
Ge-S	0.0588	−0.0043	0.0248	−0.0508	2.0430	−0.4404	0.4222	2.7262	1.4908	1.2359	1.2062	177.7
	0.0548	−0.0063	0.0217	−0.0449	2.0732	−0.4240	0.3951	2.7777	1.5133	1.2646	1.1967	178.4
	0.0541	0.0025	0.0226	−0.0446	1.9728	−0.4069	0.4183	2.7654	1.5288	1.2368	1.2361	178.6
	0.0753	0.0560	0.0479	−0.0818	1.7075	−0.4500	0.6361	2.4466	1.2631	1.1835	1.0672	179.8
Rh-Ge	0.0753	0.0343	0.0443	−0.0800	1.8066	−0.4741	0.5878	2.4659	1.2818	1.1842	1.0824	179.2
	0.0746	0.0426	0.0450	−0.0794	1.7638	−0.4612	0.6038	2.4728	1.2836	1.1892	1.0794	179.7
	0.0599	0.0694	0.0379	−0.0585	1.5423	−0.3431	0.6327	2.7223	1.4327	1.1533	1.2423	177.6
Rh-Te	0.0576	0.0581	0.0344	−0.0542	1.5772	−0.3442	0.5963	2.7400	1.4466	1.2935	1.1183	179.5
	0.0571	0.0555	0.0336	−0.0533	1.5868	−0.3449	0.5877	2.7457	1.3355	1.1702	1.1413	178.2
	0.0160	0.0316	0.0082	−0.0084	1.0331	−0.0170	0.5121	3.5861	1.6022	1.7799	0.9002	178.6
	0.0153	0.0296	0.0076	−0.0079	1.0312	−0.0156	0.4998	3.6381	1.9263	1.6176	0.8398	178.3

Table S1. *Cont.*

Ba-Te	0.0147	0.0240	0.0065	−0.0070	1.0803	−0.0357	0.4445	3.6292	1.6213	1.9127	0.8476	179.0
	0.0133	0.0226	0.0059	−0.0062	1.0434	−0.0193	0.4443	3.7224	1.6274	1.8685	0.8710	178.0
	0.0132	0.0285	0.0069	−0.0066	0.9604	0.0206	0.5212	3.6491	1.4583	1.7885	0.8154	179.4
	0.0231	0.0346	0.0112	−0.0137	1.2253	−0.1086	0.4822	3.3322	1.5333	1.5333	1.0000	180.0
	0.0145	0.0202	0.0058	−0.0066	1.1358	−0.0547	0.4030	3.7062	1.8767	1.8332	1.0237	174.9
Te-Te	0.0115	0.0171	0.0045	−0.0048	1.0575	−0.0226	0.3935	3.8645	1.9154	1.8479	1.0365	174.8
	0.0065	0.0103	0.0024	−0.0021	0.9100	0.0328	0.3646	4.4763	2.2547	2.2448	1.0044	168.4
	0.0052	0.0068	0.0016	−0.0015	0.9305	0.0210	0.3020	4.6936	2.3659	2.3625	1.0014	166.1
						$BaRh_2Ge_4S_4Te_2$						
	0.1027	0.0629	0.0751	−0.1345	1.7908	−0.5785	0.7315	2.2292	1.0227	1.2066	0.8476	179.0
	0.0744	0.0403	0.0445	−0.0789	1.7736	−0.4626	0.5979	2.4032	1.0767	1.3270	0.8114	177.9
Ge-S	0.0700	0.0636	0.0447	−0.0735	1.6441	−0.4116	0.6391	2.4276	1.0853	1.3423	0.8085	179.7
	0.0582	0.0126	0.0272	−0.0512	1.8839	−0.4130	0.4673	2.5472	1.1526	1.2906	0.8931	177.6
Te-Ge	0.0648	−0.0188	0.0269	−0.0585	2.1750	−0.4876	0.4150	2.6721	1.4742	1.1981	1.2305	179.2
	0.0815	0.1131	0.0629	−0.0975	1.5502	−0.4243	0.7712	2.4072	1.1092	1.1766	0.9428	177.9
Rh-Ge	0.0803	−0.0244	0.0388	−0.0837	2.1569	−0.5595	0.4837	2.4292	1.2607	1.1686	1.0787	178.9
	0.0767	0.0761	0.0524	−0.0859	1.6372	−0.4357	0.6837	2.4558	1.2666	1.1893	1.0650	179.0
	0.0633	−0.0134	0.0267	−0.0567	2.1253	−0.4738	0.4211	2.6871	1.4207	1.2668	1.1215	178.2
Te-Rh	0.0620	0.0468	0.0357	−0.0597	1.6720	−0.3870	0.5758	2.7013	1.4346	1.2668	1.1325	179.3
	0.0613	0.0989	0.0439	−0.0630	1.4363	−0.3121	0.7153	2.7087	1.4397	1.2690	1.1345	179.5
	0.0179	0.0450	0.0110	−0.0108	0.9796	0.0126	0.6150	3.2834	1.5272	1.5073	1.0132	178.7
	0.0176	0.0410	0.0102	−0.0102	1.0001	0.0000	0.5824	3.3375	1.5609	1.6881	0.9246	179.0
Ba-S	0.0137	0.0327	0.0077	−0.0072	0.9374	0.0352	0.5628	3.4759	1.7715	1.6161	1.0961	178.4
	0.0132	0.0302	0.0071	−0.0067	0.9421	0.0314	0.5428	3.4602	1.6212	1.7507	0.9260	178.0
	0.0112	0.0297	0.0066	−0.0057	0.8679	0.0774	0.5859	3.5452	1.6351	1.8015	0.9077	178.3
	0.0254	0.0656	0.0172	−0.0181	1.0486	−0.0330	0.6786	2.9143	1.3127	1.3127	1.0000	180.0
	0.0075	0.0119	0.0028	−0.0026	0.9427	0.0214	0.3734	3.7573	1.8478	1.9103	0.9672	177.5
S-S	0.0061	0.0126	0.0027	−0.0022	0.8265	0.0764	0.4400	3.8823	1.9145	1.9747	0.9696	173.2
	0.0040	0.0023	0.0007	−0.0008	1.1529	−0.0254	0.1662	4.4434	2.2107	2.2340	0.9896	177.1
	0.0038	−0.0003	0.0002	−0.0005	2.3778	−0.0765	0.0555	4.4187	2.1854	2.2536	0.9698	169.1

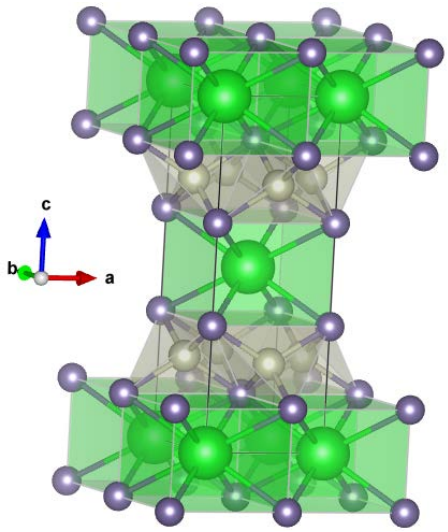

Figure S1. Structure of the $Ba_2Rh_4Ge_4$ compound. The barium atom (big, green balls) is surrounded by six germanium ones (purple), forming an inverted bipyramid (rectangular trapezoprism). The rhodium atom (kaki) is at the centre of a tetrahedron formed by four germanium atoms.

Table S2. Atomic charges borne by the Ba, Rh and Ge atoms in the $Ba_2Rh_4Ge_4$ structure.

Atom	Multiplicity in the Cell	Charge (e)
Ba	2	1.23
Rh	4	–0.56
Ge	4	–0.06