

Table 5. Selected bond critical points (BCPs) and ring critical points (RCPs) for [Rh(PR₃)(Binor-S)]⁺ [R = ⁱPr (1), R = Cy (2)]

BCP	Atoms	Signature	1			2		
			ρ_b	$\nabla^2\rho_b$	ϵ	ρ_b	$\nabla^2\rho_b$	ϵ
1	C(25)-C(21)	(3, -1)	0.1771	-0.08693	1.670742	0.1817	-0.09211	1.441
2	C(25)-C(26)	(3, -1)	0.2374	-0.4104	0.280953	0.2362	-0.4125	0.2542
3	C(21)-C(26)	(3, -1)	0.2359	-0.4015	0.281686	0.2369	-0.4041	0.2991
4	C(25)-C(21)-C(26)	(3, +1)	0.1725	0.1323	-	0.1752	0.1484	-
5	C(25)-H(25)	(3, -1)	0.2558	-0.8080	0.040093	0.2584	-0.8254	0.0388
6	C(21)-H(21)	(3, -1)	0.2563	-0.8123	0.040241	0.2609	-0.8414	0.03784
7	Rh-C(25)-C(21)	(3, +1)	0.06818	0.20130	-	0.06186	0.1854	-
8	Rh-C(25)	(3, -1)	0.07075	0.18600	0.840406	0.06404	0.1732	0.9363
9	Rh-C(21)	(3, -1)	0.07054	0.18700	0.875989	0.06328	0.1716	1.188
10	C(15)-C(16)	(3, -1)	0.2359	-0.4696	0.019244	0.2346	-0.4569	0.02707
11	C(16)-C(11)	(3, -1)	0.2376	-0.4699	0.027961	0.2357	-0.4608	0.02755
12	C(15)-H(15)	(3, -1)	0.2598	-0.8344	0.011742	0.2589	-0.8278	0.01412
13	C(11)-H(11)	(3, -1)	0.2590	-0.8308	0.010432	0.2598	-0.8327	0.01395
14	Rh-C(15)	(3, -1)	0.1294	0.07425	0.031807	0.1317	0.07908	0.0164
15	Rh-C(11)	(3, -1)	0.1280	0.07367	0.034884	0.1304	0.07574	0.00981
16	Rh-C(15)-C(11)	(3, +1)	0.06623	0.2154	-	0.0654	0.2267	-
17	C(2)-H(2a)	(3, -1)	0.246	-0.7321	0.009851	0.2516	-0.7683	0.006719
20	Rh-H(2a)	(3, -1)	0.02917	0.07906	0.679124			