

Supporting Information

**Unusual Cationic Rhodathiaboranes: Synthesis and
Characterization of [8,8,8-(H)(PR₃)₂-9-(Py)-*nido*-8,7-
RhSB₉H₁₀]⁺ and [1,3-μ-(H)-1,1-(PR₃)₂-3-(Py)-*isonido*-
1,2-RhSB₉H₈]⁺**

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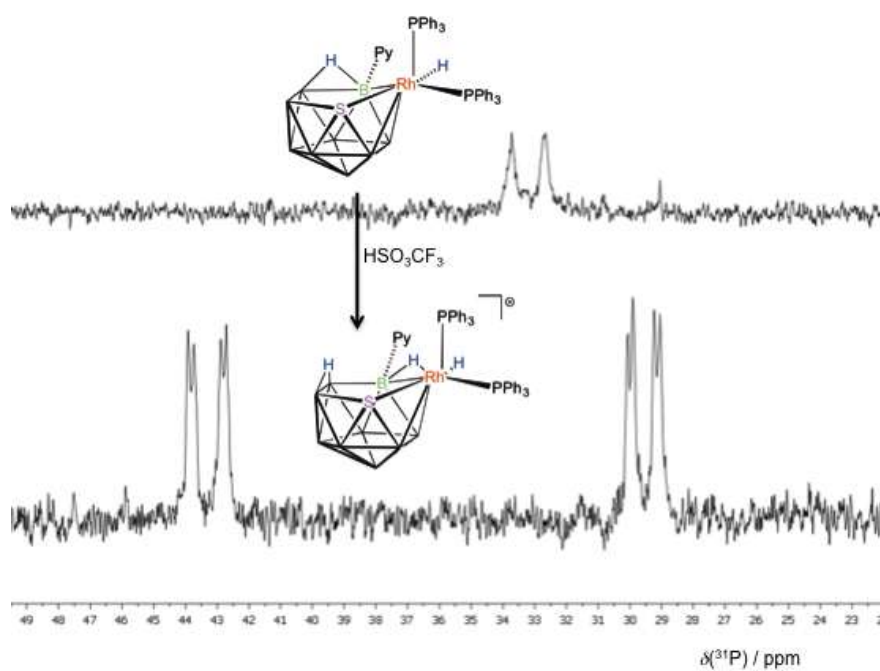


Figure S1. $^{31}\text{P}\{-^1\text{H}\}$ NMR spectra of **2** and **12**.

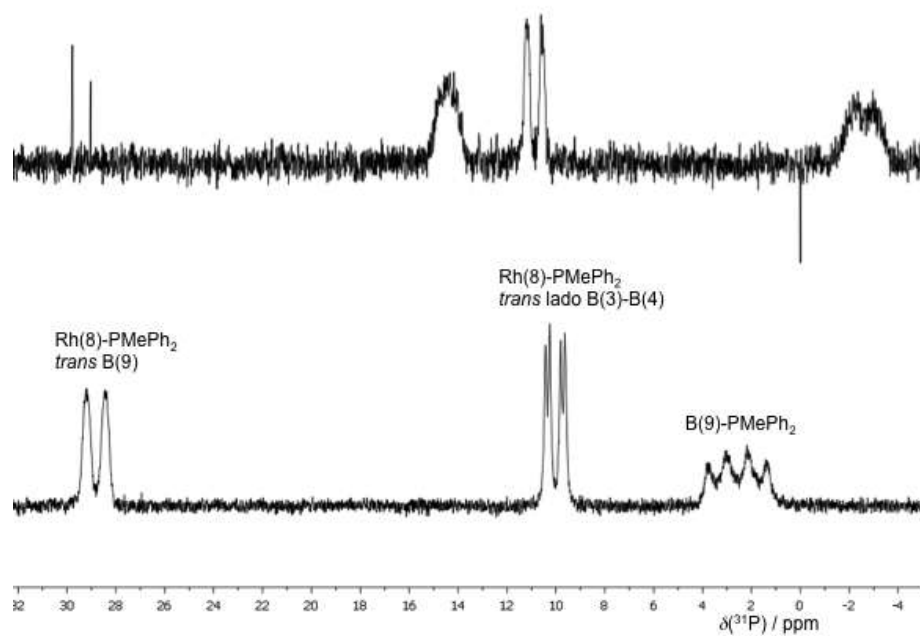


Figure S2. $^{31}\text{P}\{-^1\text{H}\}$ NMR spectra of **6** (top) and **16** (bottom).

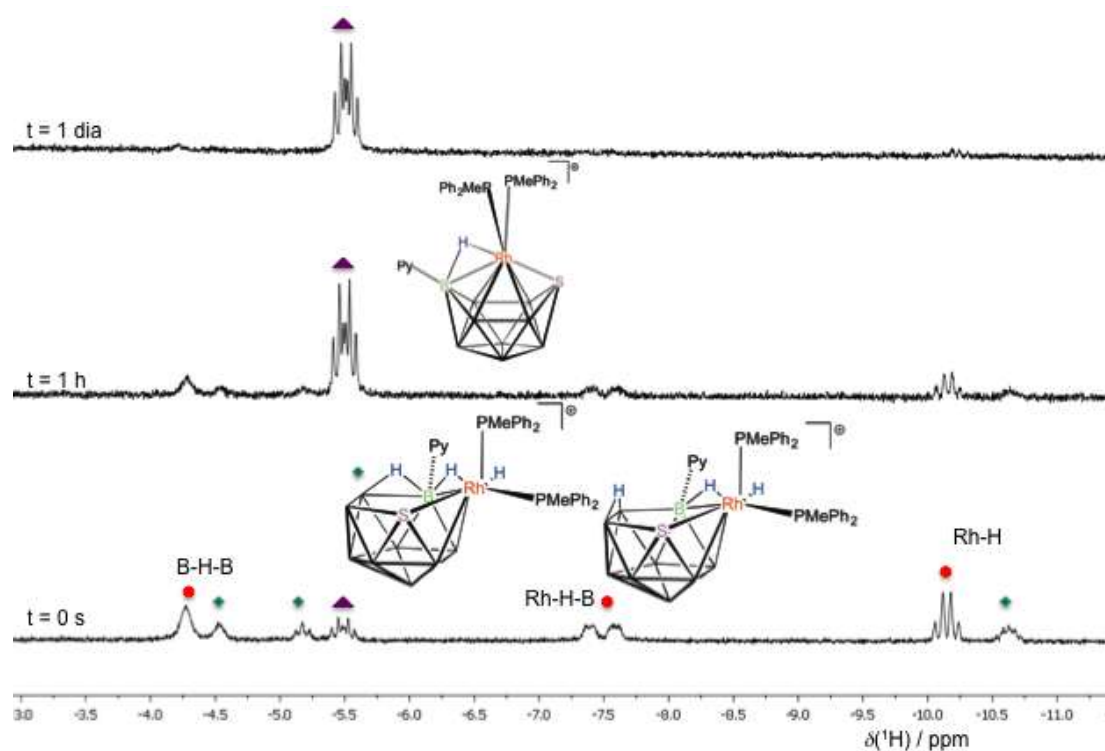


Figure S3. $^1\text{H}\{-^{11}\text{B}\}$ NMR spectra of **3** after treatment with TfOH: upon addition of acid, there is formation of two cationic *nido*-isomers (red circles and green triangles), **13**, together with small amounts of the *isonido*-cation, **22**. In one day, the reaction mixture leads to the formation of **22** as a single product.

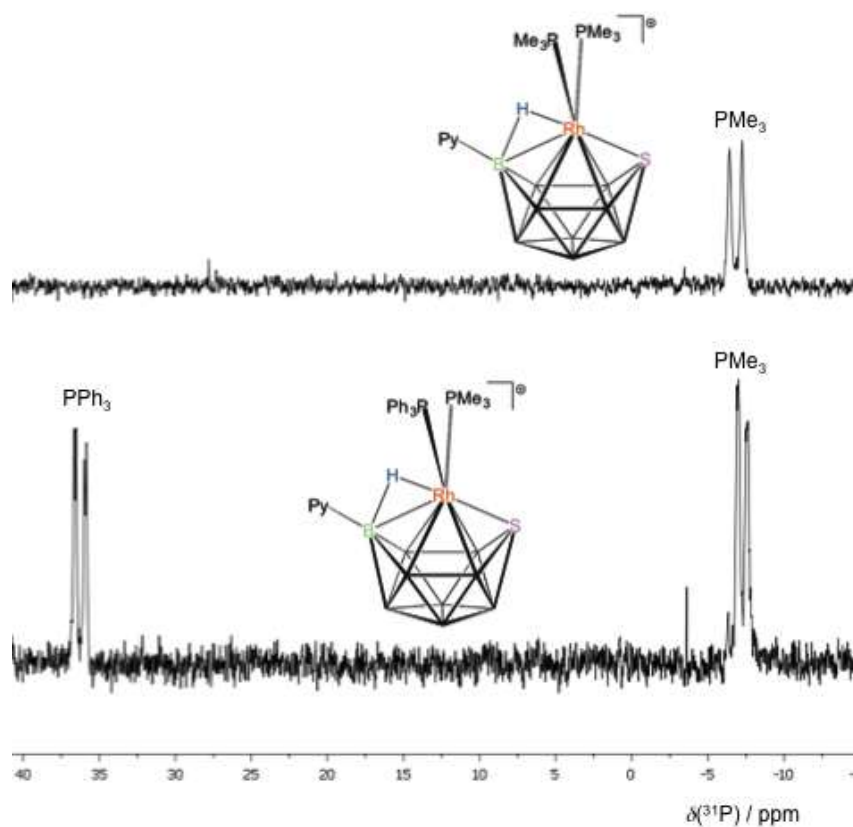


Figure S4. $^{31}\text{P}\{-^1\text{H}\}$ NMR spectra of **20** (bottom) y **19** (top).

Computational details

The geometry of all structures has been optimized with the G09 program package^[1] at the DFT level using the B3LYP approximation^[2] combined with the def2-SVP basis set for all atoms^[3] and pseudo-potentials^[4] for Rh. The nature of the stationary points has been confirmed by frequency analysis.

References for the computational study

- [1] Gaussian 09, Revision A.1, M. J. Frisch, G. W. Trucks, H. B. Schlegel, G. E. Scuseria, M. A. Robb, J. R. Cheeseman, G. Scalmani, V. Barone, B. Mennucci, G. A.

Petersson, H. Nakatsuji, M. Caricato, X. Li, H. P. Hratchian, A. F. Izmaylov, J. Bloino, G. Zheng, J. L. Sonnenberg, M. Hada, M. Ehara, K. Toyota, R. Fukuda, J. Hasegawa, M. Ishida, T. Nakajima, Y. Honda, O. Kitao, H. Nakai, T. Vreven, J. A. Montgomery, Jr., J. E. Peralta, F. Ogliaro, M. Bearpark, J. J. Heyd, E. Brothers, K. N. Kudin, V. N. Staroverov, R. Kobayashi, J. Normand, K. Raghavachari, A. Rendell, J. C. Burant, S. S. Iyengar, J. Tomasi, M. Cossi, N. Rega, J. M. Millam, M. Klene, J. E. Knox, J. B. Cross, V. Bakken, C. Adamo, J. Jaramillo, R. Gomperts, R. E. Stratmann, O. Yazyev, A. J. Austin, R. Cammi, C. Pomelli, J. W. Ochterski, R. L. Martin, K. Morokuma, V. G. Zakrzewski, G. A. Voth, P. Salvador, J. J. Dannenberg, S. Dapprich, A. D. Daniels, Ö. Farkas, J. B. Foresman, J. V. Ortiz, J. Cioslowski, and D. J. Fox, Gaussian, Inc., Wallingford CT, 2009.

[2] A. D. Becke, *Phys. Rev. A* **1988**, *38*, 3098-3100. C. Lee, W. Yang, W., R. G. Parr, *Phys. Rev. B* **1988**, *37*, 785-789. A. D. Becke, *J. Chem. Phys.* **1993**, *98*, 5648-5652.

[3] F. Weigend, R. Ahlrichs, *Phys. Chem. Chem. Phys.* **2005**, *7*, 3297-3305.

[4] K. A. Peterson, D. Figgen, E. Goll, H. Stoll, M. Dolg, *J. Chem. Phys.* **2003**, *119*, 11113-11123.

Tables of the optimized geometries (Cartesian coordinates, in Angstroms).

Energies (in Hartrees) in parenthesis.

Table S1. [8,8,8-(H)(PPh₃)₂-9-(NC₅H₅)-nido-8,7-RhSB₉H₁₀]⁺ (**12**) (-3058.85832561)

Atom	x	y	z
Rh	-0.206249479	-0.7102631308	-0.3663781811
P	-0.9415245579	1.6374707577	-0.0558738438
P	2.1038597242	-0.5628510389	0.2971285887
C	-2.4416388004	1.8745986971	-1.1222501983
C	-2.3505361331	2.4378530707	-2.4034694271
C	-3.6970163344	1.4332095238	-0.6686153653
C	-3.4849628562	2.5515789546	-3.2114671104
C	-4.829507719	1.5563738656	-1.4740681402
C	-4.7260842722	2.1119767411	-2.7517563393

C	0.1645048856	3.0166854237	-0.5874973746
C	0.1889827263	4.2589514051	0.0662544902
C	0.996369068	2.8194801831	-1.7015321536
C	1.0235607316	5.279613642	-0.3923666297
C	1.8253293034	3.8442643665	-2.1610294449
C	1.8411956855	5.0770263627	-1.5062478343
C	2.774659004	-2.2186628264	0.7692085179
C	3.9796021866	-2.6966454152	0.2327059533
C	2.0809960168	-3.0207907324	1.6912416562
C	4.483751001	-3.9395029495	0.6223353809
C	2.5963344578	-4.2524946438	2.0917970059
C	3.799654384	-4.7167922941	1.5558733135
C	3.3769904132	0.1202478704	-0.8593913765
C	4.5986645354	0.5842442736	-0.3349012818
C	3.2015806703	0.1208139589	-2.2503051974
C	5.6062313636	1.0442592925	-1.1819545102
C	4.2122607995	0.5828052769	-3.0964728023
C	5.4153727888	1.0478962415	-2.5655299327
C	-1.5450735656	2.1107264059	1.6209643965
C	-1.0325838456	1.4697086595	2.7581752574
C	-2.4902170257	3.1402278369	1.7911303236
C	-1.451264845	1.8480716748	4.0356670605
C	-2.9076817805	3.5141555065	3.0684877337
C	-2.3891761927	2.8687494534	4.1939038945
C	2.3579648235	0.4807438399	1.80955639
C	2.4490372903	1.8764598328	1.6714248543
C	2.4544623196	-0.0745700729	3.0952599617
C	2.615966968	2.6930291739	2.7897835157
C	2.6208136809	0.7468748828	4.2130109381
C	2.6973759123	2.132184759	4.0655720635
H	-0.3053112098	-0.933884346	1.1734094283
H	-1.399614359	2.8034299937	-2.7755369801
H	-3.7964623022	1.0207763905	0.3313534114
H	-3.3945462973	2.9936525053	-4.1994088096
H	-5.7964997934	1.229570931	-1.1005660098
H	-5.6072446996	2.2074648707	-3.3791666738
H	-0.4314928453	4.4325646192	0.938016239
H	1.0092621604	1.8599937333	-2.2071903139
H	1.0334735355	6.2353295011	0.124128353
H	2.4654756841	3.6710261197	-3.0209615839
H	2.4899902102	5.8736847746	-1.85854758
H	4.529471515	-2.1079311447	-0.4916611641
H	1.1285171721	-2.6866819807	2.0896347062
H	5.4146694221	-4.2962821253	0.1914026976
H	2.0509197922	-4.8567492484	2.8112551933
H	4.1955698077	-5.6816134255	1.859078268
H	4.7692488255	0.5838495722	0.7361974339
H	2.2830484063	-0.2452841329	-2.6885877703
H	6.5418553146	1.3971187316	-0.7577683042
H	4.0556683727	0.5709191263	-4.1713193542

H	6.2017087835	1.4056471202	-3.2239880362
H	-0.2988916377	0.6794025498	2.649252551
H	-2.9081281228	3.6468654677	0.9268801676
H	-1.0377339957	1.3452204545	4.9051677199
H	-3.6383357491	4.3098455138	3.1829586504
H	-2.7155489043	3.16176606	5.18777859
H	2.4130737423	2.330803577	0.6890622957
H	2.4289815224	-1.148346134	3.2344880901
H	2.6882755812	3.7687145268	2.6579981341
H	2.7071314768	0.2964006651	5.1979396726
H	2.8332487464	2.7684991404	4.9353498192
B	-0.4610960505	-3.7258310791	-2.2409700898
B	-2.1624399482	-2.1567588806	-0.4496701909
B	0.5129471259	-2.3085720414	-1.9274704588
B	-0.5440866107	-2.9678849222	-0.6007262024
B	-1.9632820576	-1.5421243744	-3.4651939929
B	-2.9993863556	-2.289090116	-2.1206432559
B	-0.3872290946	-2.5935864706	-3.5608230087
B	-2.0111034585	-3.5737579189	-1.4265911204
B	-1.9549212798	-3.2904210184	-3.17232305
S	-0.2500331259	-0.705880669	-2.9309571521
N	-3.069051813	-2.385026628	0.8202738952
C	-2.6141025706	-3.0933910885	1.8785313179
C	-4.3339700243	-1.9039182155	0.838572256
C	-3.4090548088	-3.3337203366	2.9897040473
C	-5.1755974052	-2.104715335	1.9222430991
C	-4.7104725793	-2.8320555997	3.0184912559
H	0.0698245097	-4.779250789	-2.3844773491
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H	1.6932020634	-2.3584426242	-2.0011055784
H	-0.0841260711	-3.6469712438	0.259896625
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H	-4.1802976571	-2.3782148726	-2.2498409442
H	-2.7042890354	-1.0731565153	-2.4283585204
H	0.1702646718	-2.7473646204	-4.5940804615
H	-2.6092303947	-4.5009329177	-0.9769939373
H	-2.4184480769	-4.0575260312	-3.9513726707
H	-1.6018238063	-3.4647893197	1.790390514
H	-4.646186154	-1.370165838	-0.0494792551
H	-3.0078319009	-3.9135870099	3.8133892721
H	-6.1830499377	-1.7048978231	1.8941890121
H	-5.3527965769	-3.0107628167	3.8751713129

Table S2. [8,8,8-(H)(PMe₃)(PPh₃)₂-9-(NC₅H₅)-*nido*-8,7-RhSB₉H₁₀]⁺ (**15**) (-2483.68758088)

Atom	x	y	z
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Rh	-0.3325143752	-0.6862908323	-0.3566017705
P	-0.9455414871	1.6742757778	-0.1246695074
P	1.9298236158	-0.5025185418	0.2266607687
C	-2.3712186418	2.0368009781	-1.2508949765
C	-2.2503105967	2.7947160966	-2.4235286773
C	-3.6278129998	1.4977380649	-0.9212603303
C	-3.3573815765	2.9961759032	-3.2533046106
C	-4.7310952017	1.7063796208	-1.7469540154
C	-4.5970364986	2.4518539339	-2.9216756802
C	0.3377993589	2.9201484073	-0.580611018
C	0.660536917	4.004832689	0.2500077817
C	1.0227801964	2.773932881	-1.8011118746
C	1.6401095108	4.9239686582	-0.1354746194
C	1.9868860383	3.704751671	-2.1905257837
C	2.3005719374	4.7808234375	-1.3558654581
C	-1.5878361902	2.2261119947	1.5126234075
C	-1.2717617192	1.5246549357	2.6845774964
C	-2.3866634072	3.3810586167	1.6066107433
C	-1.7343462958	1.9685882916	3.9255924545
C	-2.8479717125	3.821967269	2.8463614815
C	-2.5220637907	3.1172686421	4.008452398
H	-0.3946500468	-0.8828745304	1.1922099237
H	-1.3018336476	3.2435842755	-2.6943759166
H	-3.750202149	0.9366283775	0.0013804598
H	-3.2451763728	3.5874102147	-4.1574255061
H	-5.6983603841	1.2943064811	-1.4725936479
H	-5.4552302073	2.6117353363	-3.567478031
H	0.1498071176	4.1399616839	1.1969414914
H	0.8003778207	1.9349526612	-2.4546136817
H	1.8794752163	5.7562149811	0.520170819
H	2.4944943367	3.5862614205	-3.1436679855
H	3.0555355437	5.5013459929	-1.6562364476
H	-0.6713202439	0.6232659927	2.6241385347
H	-2.6513384136	3.9343629943	0.710767265
H	-1.4800932284	1.4152968355	4.8253389904
H	-3.463667563	4.7149067129	2.9040849791
H	-2.8833956109	3.4620487365	4.9730272826
B	-0.4832468902	-3.7499727864	-2.1415575539
B	-2.2227634644	-2.1894371176	-0.3700404864
B	0.4439249331	-2.2935958097	-1.8908473013
B	-0.5698947793	-2.9482306794	-0.5188938067
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B	-0.4622742977	-2.6527395187	-3.4946874856
B	-2.0267450834	-3.6269839377	-1.3094442533
B	-2.0005255755	-3.390420117	-3.0658646098
S	-0.3700679234	-0.7424755935	-2.9151085518
N	-3.1087240121	-2.4179734931	0.9136274527

C	-2.6351744196	-3.1206966981	1.9677570102
C	-4.3771361241	-1.9464987712	0.9467593601
C	-3.4153086988	-3.3645892695	3.0888175184
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C	-4.7202989015	-2.8735829059	3.131942636
H	0.0816029073	-4.7886884257	-2.2616599139
H	-2.1136749169	-0.9248422148	-0.5025169324
H	1.6251336522	-2.3115919322	-1.9828892446
H	-0.0651023439	-3.5786360181	0.3597525313
H	-2.542258411	-1.1999870615	-4.3924618385
H	-4.2456612108	-2.5338525042	-2.1455810288
H	-2.8193677738	-1.1827958282	-2.3716754588
H	0.090483075	-2.8166563406	-4.5286060011
H	-2.5863737061	-4.5642923922	-0.8326567655
H	-2.4443446421	-4.1942120836	-3.8186074338
H	-1.6202343886	-3.483068395	1.8708935115
H	-4.7065315124	-1.4200308711	0.0603228599
H	-2.9993428518	-3.9395179167	3.9086443677
H	-6.2150970381	-1.7591768869	2.0233361778
H	-5.3512408703	-3.0563182722	3.9961737417
C	2.3004564628	0.6823717063	1.58858962
H	2.0272620002	1.7007596248	1.3024932998
H	1.7443167999	0.4058536157	2.4880726814
H	3.3722665987	0.6556057446	1.8136676348
C	2.6042309697	-2.078091595	0.896570358
H	2.020705965	-2.3767365457	1.7714235195
H	2.5358536989	-2.8711023853	0.1492952154
H	3.6510481839	-1.941013131	1.1882826065
C	3.1421547743	-0.0097955208	-1.0701784358
H	2.9539574623	1.0203366716	-1.3807451314
H	4.1564834496	-0.0785548704	-0.6611767496
H	3.062878052	-0.665793418	-1.9391301362

Table S3. [8,8,8-(H)(PMePh₂)₂-9-(PMePh₂)-nido-8,7-RhSB₉H₁₀]⁺ (**16**) (-3271.67236962)

Atom	x	y	z
Rh	0.3797308498	-0.1127834223	-0.2503089834
B	-0.8070528647	-2.0872400897	-2.9499503758
B	-1.9660581981	-0.2311263497	-0.9867117715
B	0.6083398149	-1.5042516343	-2.1037043369
B	-0.945608061	-1.7443538346	-1.1752880514
B	-0.6742709681	0.7478348384	-3.6296943625
B	-2.2602219062	0.4288196461	-2.717472234
B	0.1528072641	-0.9441225206	-3.8477240973
B	-2.2395289482	-1.2945613076	-2.32612595

B	-1.5898753202	-0.7479213369	-3.8833893744
S	1.0282868556	0.411147541	-2.6723612444
P	0.7985564125	1.9976659226	0.913809808
P	2.3079307804	-1.2140002441	0.5886098392
P	-3.4969691987	-0.0050342025	0.2323921442
C	-5.0306177071	-0.8631347676	-0.2761432235
C	-5.5801433425	-1.8989822708	0.4932518896
C	-5.6775003698	-0.4617996663	-1.4584290472
C	-6.7601300543	-2.5232531027	0.0846622415
C	-6.8559353053	-1.0885348683	-1.8579481455
C	-7.3988610536	-2.1201733495	-1.0879422828
C	-3.1605853803	-0.4942748721	1.9598122049
C	-3.529736705	0.321383576	3.0411691242
C	-2.5582147122	-1.7395773026	2.2111572743
C	-3.2944342781	-0.0993279682	4.3522926258
C	-2.3398003789	-2.1606313701	3.523333
C	-2.7026397244	-1.3400206046	4.5948815565
C	-3.9443563331	1.775423464	0.2566636665
H	-0.1761775031	-0.6313118819	1.1122947955
H	-0.8301415827	-3.2079306199	-3.3449698027
H	1.5801269257	-2.1774406356	-2.0550867103
H	-1.0991072206	-2.7177299259	-0.5083997328
H	-0.5615482287	1.5846827878	-4.4633135723
H	-3.2410534064	1.0241589198	-3.0382243192
H	0.8158619624	-1.1792384503	-4.8006036424
H	-3.2956176774	-1.836532798	-2.2905957645
H	-2.1436090904	-0.9757657797	-4.9091978808
H	-5.0994155697	-2.2183373555	1.4112433627
H	-5.2607868676	0.325347693	-2.0783234838
H	-7.1784935873	-3.3236380399	0.6877012978
H	-7.3466782895	-0.7733051222	-2.7738622957
H	-8.3168260476	-2.6076666897	-1.4028456141
H	-4.0085536641	1.2806313778	2.8740872656
H	-2.2655439994	-2.3760102911	1.3819353015
H	-3.5851845097	0.5387783569	5.1816671412
H	-1.8892760744	-3.1314415526	3.7095302082
H	-2.5312574605	-1.670113116	5.6153695702
H	-4.155933635	2.0864220382	-0.7692986583
H	-4.833989957	1.9499206481	0.8670418524
H	-3.1092051673	2.3758363106	0.6271110044
H	-1.3393615571	1.3208329098	-2.5910159973
C	-0.182566271	3.3962540962	0.2040227595
C	-0.0556990658	3.6937265064	-1.163188798
C	-1.0306517401	4.1935913751	0.989484069
C	-0.7540356417	4.7596376046	-1.7294916876
H	0.5996835351	3.0994377105	-1.7916479318
C	-1.7348522122	5.2576846985	0.4181834024
H	-1.1462961555	4.0055417699	2.0513576639

C	-1.5992730308	5.5433230803	-0.9402624429
H	-0.6366231968	4.9766863026	-2.7872043353
H	-2.3824992815	5.8671047185	1.0422757162
H	-2.1440154905	6.3729859851	-1.3810668408
C	2.5093714485	2.6784084072	0.9711397721
C	3.0471719194	3.265629543	2.1279293931
C	3.2775694083	2.6645337622	-0.2045556766
C	4.3233111532	3.8321054456	2.1035025833
H	2.4796752674	3.2972437166	3.0520812648
C	4.5449085933	3.2450535354	-0.2291509642
H	2.8923822086	2.1910169092	-1.102459524
C	5.0707406913	3.8293101503	0.9250544556
H	4.7268647505	4.2831434455	3.0055771761
H	5.1246689853	3.2290007101	-1.1470850878
H	6.0595913094	4.278306664	0.9069471669
C	2.2201564436	-3.0518722157	0.5476024553
C	3.2481171006	-3.8364214053	0.0062563137
C	1.1135877428	-3.682780009	1.138241474
C	3.1664403032	-5.2299345554	0.054957038
H	4.1128297191	-3.369461898	-0.4518383098
C	1.0415096635	-5.0734131795	1.1923960999
H	0.3015414067	-3.0863488152	1.5426385878
C	2.0667006093	-5.8503921557	0.6470637302
H	3.9664526493	-5.827701767	-0.3720010001
H	0.1804529188	-5.5520920478	1.650239546
H	2.0056553245	-6.9342023151	0.6821292639
C	3.954763788	-0.778582655	-0.1125190888
C	5.0223728853	-0.421995756	0.7286761239
C	4.1815463867	-0.8288643203	-1.4998457718
C	6.2783636763	-0.1242486139	0.1976220319
H	4.8925775581	-0.3704692282	1.8029068449
C	5.4385836172	-0.532361591	-2.0264455355
H	3.3856607769	-1.1141510897	-2.1759162566
C	6.4910213662	-0.1778012902	-1.1798023544
H	7.0899250874	0.1468819264	0.866640043
H	5.5931971371	-0.5840132381	-3.10029242
H	7.4702303348	0.0500807112	-1.5909834278
C	0.2488609519	1.9329042661	2.6748095666
H	-0.7931011297	1.6044742952	2.7067886525
H	0.8463774154	1.195841266	3.2139976236
H	0.3381193489	2.8969891769	3.1820069117
C	2.5063705349	-0.9224935709	2.4043116458
H	2.7498790068	0.1224809696	2.6106767286
H	1.5654875553	-1.1789848239	2.8962099631
H	3.295020428	-1.5642347605	2.806330913
H	-1.1838639912	0.7142044566	-0.6322606162

Table S4. [1,3- μ -(H)-1,1-(PMe₃)(PPh₃)₂-3-(NC₅H₅)-isonido-8,7-RhSB₉H₈]⁺ (20) (-2482.48787842)

Atom	x	y	z
H	1.19070600	0.37188800	-1.04009600
C	-1.04496000	1.53514300	2.75436300
H	-0.20083200	2.07555800	2.33982300
Rh	0.68243600	-0.83237800	-0.18321700
P	0.16470500	-1.68219100	-2.37886100
P	-1.35216300	0.51936000	0.15720600
N	3.36205700	1.09578300	-0.02543200
S	-0.06389900	-2.79831700	1.09784000
B	3.02806100	-2.87600100	1.35774700
H	3.92521400	-3.65642400	1.40158000
B	1.55574000	-3.31948000	2.17219300
H	1.35138000	-4.32886500	2.75561200
B	1.68376600	-3.16318100	0.29078600
H	1.61724100	-4.07265900	-0.47071500
B	2.87589100	-1.79597200	-0.07067900
H	3.56336900	-2.00453400	-1.02457500
B	3.42198100	-1.16896900	1.53408900
H	4.52343000	-0.81460800	1.82356100
B	2.35900800	-1.88068300	2.74666600
H	2.75202100	-1.84703200	3.86964000
B	2.57622400	-0.16113900	0.43850300
B	1.84470700	-0.33176100	1.97417400
H	1.72521300	0.63814400	2.65921500
B	0.66159700	-1.69629500	2.49383600
H	-0.11767000	-1.47627800	3.35779200
C	2.86637300	2.33672400	0.19607800
H	1.88740000	2.37506900	0.65429000
C	3.57664100	3.47477600	-0.14846500
H	3.14493200	4.44943900	0.04928600
C	4.83603800	3.34011100	-0.73748200
H	5.41330700	4.21743200	-1.01214100
C	5.34129800	2.05963200	-0.96282500
H	6.31538200	1.90558700	-1.41339700
C	4.58442600	0.95757700	-0.59286400
H	4.92650500	-0.05963700	-0.73081400
C	-1.23284900	2.27309700	-0.42082100
C	-0.39542600	2.63240800	-1.48751300
H	0.23809300	1.88408600	-1.95136400
C	-0.36404400	3.94508100	-1.96337800
H	0.28826800	4.20147300	-2.79368200
C	-1.17012400	4.92187200	-1.37686900
H	-1.14624400	5.94349400	-1.74498900
C	-2.00999800	4.57804200	-0.31530100
H	-2.64220500	5.33079100	0.14660700
C	-2.04457000	3.26601900	0.15858100

H	-2.70479200	3.01688000	0.98235900
C	1.68367900	-2.09587600	-3.33517200
H	2.24191900	-2.88593900	-2.82924600
H	2.32899500	-1.21673400	-3.41500200
H	1.40834700	-2.43307700	-4.34063300
C	-0.72263000	-0.56547100	-3.54880600
H	-0.86706400	-1.07661000	-4.50685600
H	-0.13311800	0.33949700	-3.72120700
H	-1.69770300	-0.27871500	-3.14903200
C	-0.81168600	-3.24225500	-2.48250000
H	-0.84357500	-3.58783700	-3.52169200
H	-1.83262900	-3.06779100	-2.13632900
H	-0.35168400	-4.01776000	-1.86495500
C	-2.88927800	-0.11103400	-0.65667300
C	-3.71678900	0.71353100	-1.43560800
H	-3.46490400	1.75723600	-1.58631800
C	-4.87716400	0.20111400	-2.02215800
H	-5.50414400	0.85303300	-2.62361700
C	-5.23475700	-1.13370500	-1.83123900
H	-6.14091800	-1.52667300	-2.28268600
C	-4.42175800	-1.96236300	-1.05379700
H	-4.69522300	-3.00133600	-0.89260000
C	-3.25299700	-1.45863000	-0.48086300
H	-2.63092200	-2.11890200	0.11626200
C	-1.82748800	0.70640500	1.93108700
C	-2.92198900	0.03322900	2.49374300
H	-3.56009000	-0.59404400	1.88224300
C	-3.21761300	0.17806700	3.85131500
H	-4.06995200	-0.34845900	4.27072800
C	-2.43223300	0.99840400	4.66049400
H	-2.66543000	1.10971300	5.71529800
C	-1.34739500	1.68238000	4.10606600
H	-0.73352200	2.32836000	4.72690700

Table S5. [9,10- μ -(H)-8,8-(PMe₃)(PPh₃)₂-9-(NC₅H₅)-*nido*-8,7-RhSB₉H₈]⁺ (20) (-2482.49162720)

Atom	x	y	z
H	2.4515542812	-0.3048664071	0.8827784222
C	-0.2165188603	1.0257018939	3.3144517378
H	0.6276862161	1.410734416	2.7476288696
Rh	0.3436972702	-0.9702676096	-0.2409317707
P	-0.3379942218	-0.7090036064	-2.4808903036
P	-1.355942895	0.5468434491	0.8012454079
N	3.0655742532	0.4693195558	-1.2549324709
S	0.6726538972	-2.0508725894	1.9641475142
B	2.632439934	-3.5717754086	0.0797862062

H	2.9367133869	-4.6359485532	-0.3528332481
B	2.0267115033	-3.5006859339	1.7341662831
H	1.8194921628	-4.4360829032	2.4302678839
B	0.9491950642	-3.1319053185	0.2500137691
H	0.0087052392	-3.8239415323	0.0220825038
B	1.9822103767	-2.3283598289	-1.0084367401
H	1.9197785948	-2.6224619115	-2.1620391778
B	3.5962241364	-2.1214228654	-0.2896799207
H	4.5829752102	-2.1888915979	-0.9543225664
B	3.5739562758	-2.7379910455	1.3783385141
H	4.5945439769	-3.1309505549	1.8446475259
B	2.5154505483	-0.7359683879	-0.4283912961
B	3.5137622525	-0.9951433617	1.0976805175
H	4.4038700766	-0.2454032139	1.347173871
B	2.5330134798	-1.8675809162	2.4377459511
H	2.7092200854	-1.6691029475	3.593106396
C	2.8658469348	1.7393798615	-0.825246071
H	2.2467587286	1.8515613699	0.0555041954
C	3.4247781637	2.8259652223	-1.4770417433
H	3.2462825648	3.8235113286	-1.0915380567
C	4.2161155639	2.6089816986	-2.6078379847
H	4.672034053	3.4435768956	-3.1311779039
C	4.4175073711	1.3003506295	-3.046645046
H	5.0300528194	1.0813003453	-3.914092803
C	3.8354240963	0.2520127899	-2.3487411652
H	3.9818673927	-0.7835282377	-2.6240676271
C	-1.2962492645	2.3547858563	0.4370123797
C	-0.5112030675	2.8438478202	-0.6166358516
H	0.064110786	2.1470227594	-1.2178596075
C	-0.4570551495	4.2122066026	-0.892535146
H	0.1509026392	4.5759195227	-1.7168050326
C	-1.1842627212	5.1108789943	-0.1106912802
H	-1.1433994695	6.175408174	-0.3221163732
C	-1.9590590765	4.6373964499	0.9513854302
H	-2.5188334911	5.3329210226	1.5698295857
C	-2.0115474587	3.2712163417	1.2285660854
H	-2.6015846655	2.9185727877	2.0690142283
C	0.8600828363	-0.4214558375	-3.8576324213
H	1.6599952341	-1.1629594414	-3.8275359624
H	1.2928654639	0.5810679306	-3.7875712933
H	0.3365529733	-0.5055413434	-4.8159429622
C	-1.683233844	0.4668743068	-2.9589607758
H	-1.9994876244	0.2509909487	-3.9854636325
H	-1.3408942485	1.5029248376	-2.9077499909
H	-2.5427963637	0.3538241294	-2.2950094939
C	-1.1032523291	-2.3311902063	-2.9196603796
H	-1.4619497544	-2.3083220269	-3.9549104914
H	-1.9508865303	-2.5237525424	-2.2556209737

H	-0.3743345149	-3.1358757652	-2.8031183222
C	-3.0442051195	-0.0341042488	0.3432115399
C	-4.1012840842	0.825739932	0.0101225691
H	-3.9551130386	1.9009473155	0.0131516485
C	-5.3511709799	0.3038930192	-0.334368697
H	-6.161059292	0.9801519687	-0.5925636366
C	-5.5614222452	-1.0760295415	-0.3431152199
H	-6.5353340319	-1.4768625075	-0.6081887525
C	-4.5152796552	-1.9406411866	-0.0098574934
H	-4.6729978652	-3.015385927	-0.0095656946
C	-3.262500065	-1.4243668444	0.3232391466
H	-2.4548118599	-2.1063130511	0.5812451323
C	-1.3529332351	0.5357133545	2.647276147
C	-2.4267554585	0.0444189724	3.4018601703
H	-3.314506007	-0.3371427891	2.9093197944
C	-2.3635608812	0.0448125712	4.7984684746
H	-3.2026126768	-0.3391037609	5.3714753418
C	-1.2337554159	0.5344815716	5.4523008891
H	-1.1870261106	0.5314978969	6.5372650448
C	-0.1589991249	1.0278165723	4.7064279391
H	0.7248578543	1.4097936368	5.2089272636