Supplementary Information for

Electrochemical Reactions of Pincer-PCP Rhodium(I) Complexes

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S1 Electrochemical data

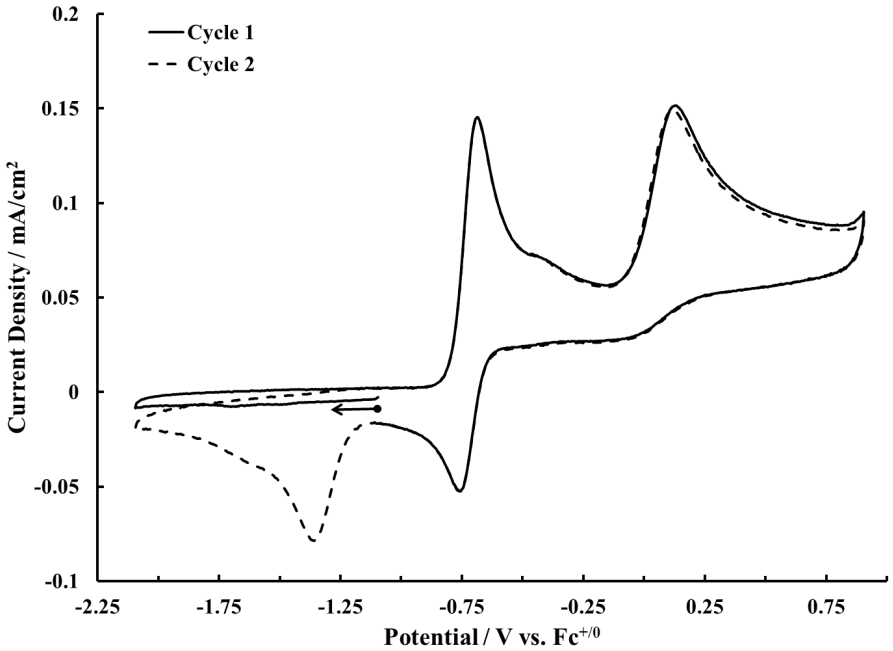

Figure A.1: CV of **1-solv** upon cycling in MeCN with 0.1 M TBAT as supporting electrolyte and at a scan rate of 0.1 Vs^{-1}.

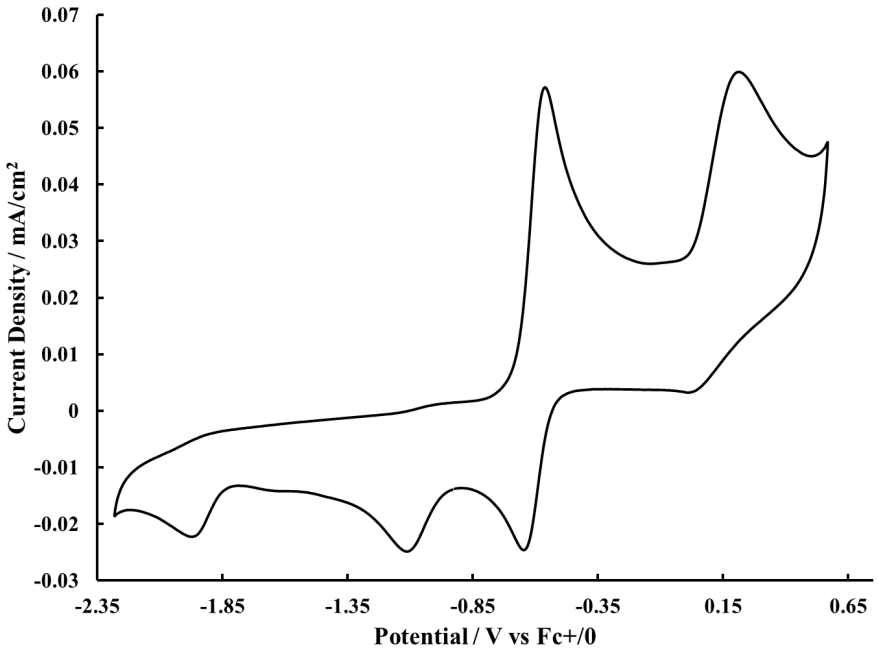

Figure A.2: CV of **1-solv** in DMSO containing 0.1 M TBAT as supporting electrolyte at a scan rate of 0.1 Vs^{-1}.

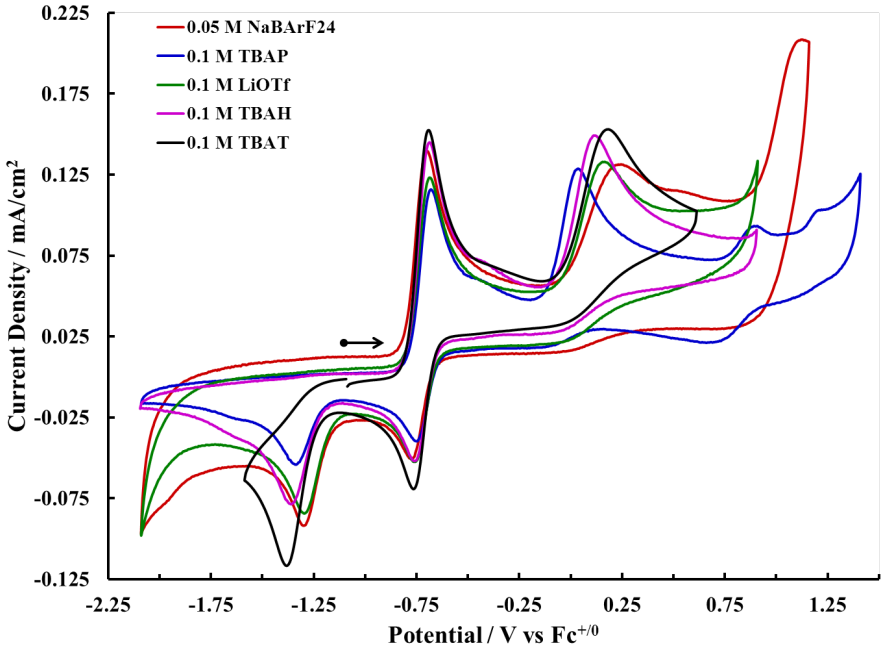

Figure A.3: CV scans of **1-solv** in MeCN with the indicated supporting electrolyte at a scan rate of 0.1 Vs^{-1}.

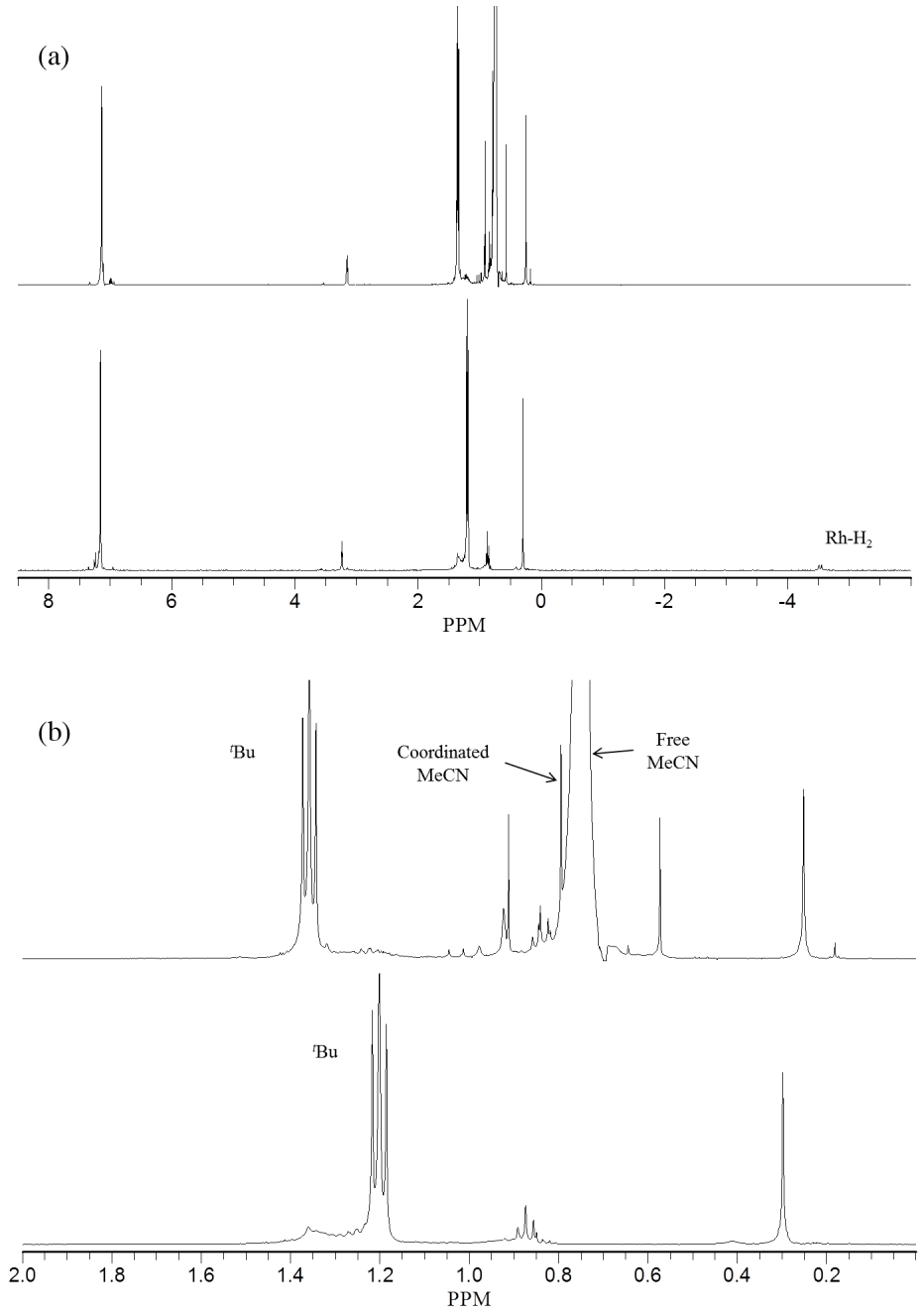

Figure A.4: ^{1}H NMR spectra of **1-H**$_2$ (bottom) and **1-H**$_2$ + CH_3CN (top) in C_6D_6 from 8.5 to -6.0 ppm (a) and 2.0 to 0.0 ppm (b).

S2 Geometries in cartesian coordinates

Table A.1: Optimized geometries obtained at the UB3LYP/LACVP/6-311G* level of theory.

1-solv

Atom	x (Å)	y (Å)	z (Å)
Rh	0.0002613243	-0.2462618373	0.4208072385
P	-2.3225797863	-0.4819898805	0.2037043013
P	2.3222137944	-0.4788817113	0.1972465698
C	1.1999431997	-4.1031698600	-1.2748898452
C	1.2034244449	-2.8610681167	-0.6343219091
C	0.0007211486	-2.1639350089	-0.3385178962
C	-1.2010033072	-2.8606024576	-0.6387717569
C	-1.1949522377	-4.1028683559	-1.2792826014
C	0.0030243194	-4.7221184584	-1.6192232787
H	2.1439795912	-4.5960110354	-1.4997610600
H	-2.1381413601	-4.5955787712	-1.5075872431
H	0.0039846611	-5.6823607092	-2.1265403356
C	2.5270831827	-2.2884030904	-0.1771291273
C	-2.5269808810	-2.2887163060	-0.1863232795
H	2.8203837908	-2.7779734042	0.7567854222
H	3.3386281798	-2.4826659831	-0.8853623951
H	-2.8284291936	-2.7860783400	0.7408926870
H	-3.3335610910	-2.4752895052	-0.9022734115
C	-3.4600422739	-0.2400416693	1.7354131744
C	-4.8273250891	-0.9436026192	1.6493738486
H	-4.7348766889	-2.0164582566	1.4687825147
H	-5.3552985698	-0.8251029340	2.6030854613
H	-5.4705348540	-0.5292211119	0.8738776260
C	-2.6725070650	-0.8426947389	2.9189768281
H	-1.7033594183	-0.3575718789	3.0468886615
H	-3.2507699516	-0.7184283186	3.8423820636
H	-2.4839541875	-1.9117808544	2.7938693063
C	-3.6795227809	1.2566231804	2.0178327428
H	-4.3484837333	1.7227097804	1.2911593600

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-4.1411558525	1.3811978605	3.0048555806
H	-2.7385443913	1.8101878431	2.0223894603
C	-3.0591398966	0.4035520772	-1.3351763664
C	-4.5745391902	0.2384367262	-1.5304650761
H	-5.1548777636	0.7767449883	-0.7784247440
H	-4.8620326098	0.6479491340	-2.5063141600
H	-4.8891740883	-0.8080583478	-1.5185549435
C	-2.7094679931	1.9016750893	-1.2723735643
H	-3.0286860878	2.3881531512	-2.2027200670
H	-3.2062550794	2.4209838775	-0.4517553011
H	-1.6337669172	2.0462091199	-1.1573893816
C	-2.3329039204	-0.1938046204	-2.5584016626
H	-1.2491557135	-0.1271417879	-2.4479139771
H	-2.5824259305	-1.2428460740	-2.7272648842
H	-2.6259257716	0.3620894350	-3.4572908968
C	3.0618710486	0.3930031390	-1.3469086355
C	2.3402791984	-0.2151311068	-2.5675589373
H	2.5917825621	-1.2651308253	-2.7269181817
H	1.2560780573	-0.1491344293	-2.4616791124
H	2.6354014929	0.3336628081	-3.4700593304
C	2.7110108947	1.8914163274	-1.2971542795
H	3.2054685006	2.4176900961	-0.4795881819
H	3.0313932979	2.3706616632	-2.2308741604
H	1.6348349128	2.0356314213	-1.1850155598
C	4.5781059995	0.2256708672	-1.5345207172
H	4.8711333156	0.6298664071	-2.5106851240
H	5.1551626516	0.7665083011	-0.7821115678
H	4.8915014192	-0.8211766383	-1.5154504003
C	3.4570917697	-0.2238977910	1.7283905948
C	2.6633603644	-0.8095788514	2.9161863144
H	1.6936501619	-0.3222918096	3.0308217487
H	2.4751789114	-1.8801809406	2.8039782953
H	3.2363523568	-0.6729224960	3.8412876357

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	4.8211869815	-0.9351469707	1.6545100571
H	5.4686123676	-0.5345682083	0.8749600492
H	5.3474196045	-0.8071689049	2.6078915252
H	4.7231587622	-2.0096528004	1.4878037358
C	3.6824210527	1.2746797162	1.9940253529
H	4.1494105414	1.4073517869	2.9770360068
H	4.3485072658	1.7315507440	1.2593127023
H	2.7432081254	1.8311903400	1.9976076603
N	-0.0001230966	1.6870564592	1.2322744535
C	-0.0022103635	2.7438470169	1.7007752857
C	-0.0066079354	4.0803225712	2.2734727657
H	-0.0102548766	4.8236569369	1.4726253849
H	0.8794841420	4.2315661903	2.8949176785
H	-0.8928025987	4.2247377292	2.8964329250
N	-0.0133612122	5.3834968047	-0.8698190714
C	-0.0089507132	4.9905248574	-1.9525493801
C	-0.0033613669	4.4866718367	-3.3181607964
H	-0.8872701881	3.8713454673	-3.4950608237
H	0.8838230842	3.8743120409	-3.4889699995
H	-0.0022905408	5.3147682078	-4.0295949944

1-solv^{+}

Atom	x (Å)	y (Å)	z (Å)
Rh	-0.0007223563	-0.2003164382	-0.1243730995
P	-2.3859243871	0.0904531171	-0.0821831816
P	2.3850017053	0.0887132458	-0.0822093378
C	1.1998144202	3.9727646499	-0.4293578817
C	1.2100236544	2.5756781437	-0.4254562713
C	0.0000972179	1.8454394674	-0.3701950873
C	-1.2090587014	2.5771206539	-0.4226708748
C	-1.1971943079	3.9742098716	-0.4264914893
C	0.0017234076	4.6741402191	-0.4107263999
H	2.1395033554	4.5167736740	-0.4582779717

Continued on Next Page...

Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-2.1363134946	4.5193184050	-0.4534053342
H	0.0023464537	5.7585953624	-0.4057949832
C	2.5357818838	1.8668822975	-0.5744527823
C	-2.5360604159	1.8701688455	-0.5692997977
H	2.8320977174	1.8927495869	-1.6263652080
H	3.3386016563	2.3677765903	-0.0287160756
H	-2.8358177967	1.8995410017	-1.6201893996
H	-3.3364621513	2.3704869609	-0.0194971394
C	-3.4045646082	-0.8536164739	-1.3847435170
C	-4.7552061842	-0.1886083617	-1.7061968285
H	-4.6473264645	0.8304776970	-2.0799122841
H	-5.2550697890	-0.7610232396	-2.4935706068
H	-5.4307012338	-0.1628722649	-0.8526233162
C	-2.5316451881	-0.8554880687	-2.6574161472
H	-1.5929861554	-1.3942154603	-2.5063627769
H	-3.0700090834	-1.3543398442	-3.4687000600
H	-2.2882758957	0.1502450318	-3.0074810768
C	-3.6431120493	-2.3078387348	-0.9494406716
H	-4.3610116667	-2.3834220446	-0.1319903794
H	-4.0556571091	-2.8743583122	-1.7893723121
H	-2.7196857178	-2.8027557453	-0.6434611366
C	-3.1048189698	-0.0143814967	1.6774610044
C	-4.6164354415	0.2524935947	1.7339232605
H	-5.1972935029	-0.5472257004	1.2737840174
H	-4.9334166888	0.3141931101	2.7792729347
H	-4.8991700481	1.1946847689	1.2603436884
C	-2.7959421240	-1.3909342566	2.2924849262
H	-3.1335969438	-1.4037201623	3.3329032490
H	-3.3036218234	-2.2081952349	1.7810309421
H	-1.7252828414	-1.6036610822	2.2937235938
C	-2.3681348150	1.0550252133	2.5107198548
H	-1.2851554735	0.9107176103	2.5052691895
H	-2.5657155926	2.0729195294	2.1736848746

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-2.7003296926	0.9873504508	3.5506568888
C	3.1035001350	-0.0112462965	1.6779848741
C	2.3679578982	1.0614021731	2.5078588463
H	2.5673347701	2.0780079873	2.1680723338
H	1.2848393460	0.9186463648	2.5019675589
H	2.6993253665	0.9962453146	3.5481527610
C	2.7929966919	-1.3855303206	2.2972158015
H	3.2992111722	-2.2050019218	1.7878971807
H	3.1311330325	-1.3959479225	3.3374579407
H	1.7220218368	-1.5965857480	2.2995769758
C	4.6153746862	0.2543129170	1.7340771618
H	4.9322027247	0.3180527049	2.7792960704
H	5.1955545786	-0.5469426388	1.2758394304
H	4.8989935571	1.1952717302	1.2586503533
C	3.4045593458	-0.8586966908	-1.3816488018
C	2.5317382895	-0.8662288462	-2.6543431194
H	1.5942474820	-1.4064673045	-2.5016589325
H	2.2861585377	0.1379629062	-3.0071505257
H	3.0709509141	-1.3660956181	-3.4643914863
C	4.7540546240	-0.1922212187	-1.7048292122
H	5.4281145002	-0.1614734371	-0.8503486217
H	5.2561499464	-0.7670248798	-2.4890972119
H	4.6445811930	0.8251560649	-2.0830399737
C	3.6461366334	-2.3109475105	-0.9413941839
H	4.0615121188	-2.8788345743	-1.7790569981
H	4.3629151498	-2.3823036237	-0.1226499387
H	2.7235591228	-2.8074015614	-0.6354574616
N	-0.0010660350	-2.3759468047	0.1501173639
C	-0.0000175685	-3.5179615061	0.2970327187
C	0.0011696755	-4.9576540489	0.4838154149
H	-0.8945309300	-5.2701483181	1.0237207646
H	0.8785307999	-5.2642041898	1.0562891398
H	0.0206324056	-5.4633129023	-0.4834018465

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)

***cis*-2^{+}**

Atom	x (Å)	y (Å)	z (Å)
Rh	0.0194142068	-0.1651210982	0.7191557973
P	-2.3676463833	-0.3039928943	0.2916411260
P	2.3998536117	-0.2808439599	0.2515225474
C	1.2211875908	-3.9193690826	-1.1366080998
C	1.2321386667	-2.6821301993	-0.4867451555
C	0.0209086404	-2.0220336397	-0.1778231335
C	-1.1888798512	-2.6932736015	-0.4677840155
C	-1.1768264064	-3.9302496320	-1.1180810642
C	0.0223274198	-4.5384279399	-1.4661762385
H	2.1609215930	-4.4055612752	-1.3832532573
H	-2.1158878246	-4.4249331587	-1.3501058064
H	0.0226527073	-5.4939037362	-1.9794326232
C	2.5632840768	-2.0980633152	-0.0640389265
C	-2.5184151485	-2.1223079175	-0.0231551683
H	2.8697164552	-2.5534083281	0.8830546512
H	3.3600155653	-2.3234475467	-0.7776218556
H	-2.8050166617	-2.5813393717	0.9283893863
H	-3.3245352447	-2.3547604652	-0.7238736927
C	-3.6743321213	0.0719343308	1.6376077343
C	-5.0166241454	-0.6439633691	1.3978428350
H	-4.9057689613	-1.7283300375	1.3395607375
H	-5.6840354088	-0.4396001984	2.2411747970
H	-5.5290972031	-0.3113217850	0.4983884394
C	-3.0965833685	-0.4281440756	2.9742088260
H	-2.1682185620	0.0793924101	3.2332143567
H	-3.8226052116	-0.2385335984	3.7709911437
H	-2.9010022668	-1.5023577632	2.9672618404
C	-3.9027756656	1.5875757450	1.7591156811
H	-4.4223861461	2.0079061958	0.8986439568
H	-4.5239097487	1.7907613327	2.6367587907

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-2.9644764750	2.1308173390	1.8901053447
C	-2.8345333608	0.5409683221	-1.3627316919
C	-4.3350045160	0.5002116576	-1.6919500184
H	-4.9376063676	1.1106434165	-1.0203908529
H	-4.4868968097	0.8966950020	-2.7005470558
H	-4.7378318480	-0.5146379819	-1.6885942056
C	-2.3450272434	2.0004923859	-1.3333650704
H	-2.5503840225	2.4728745098	-2.2986575040
H	-2.8395874462	2.6004619034	-0.5696136375
H	-1.2685079821	2.0593444562	-1.1612038619
C	-2.0843092484	-0.1953519156	-2.4882551872
H	-1.0109486563	-0.2414692247	-2.3130605949
H	-2.4380311879	-1.2163991650	-2.6339756402
H	-2.2428344656	0.3398068644	-3.4292892745
C	2.8272048822	0.5671535499	-1.4121185529
C	2.0669310920	-0.1802335660	-2.5235404087
H	2.4311621723	-1.1969113635	-2.6738032111
H	0.9973919469	-0.2399510900	-2.3301417309
H	2.2025842925	0.3553404100	-3.4679156863
C	2.3203381077	2.0206895991	-1.3760770899
H	2.8200881086	2.6275617787	-0.6211844196
H	2.5041633740	2.4944587763	-2.3450265443
H	1.2461773473	2.0668770738	-1.1863727143
C	4.3220421613	0.5452576497	-1.7678221096
H	4.4508574048	0.9412402446	-2.7798704345
H	4.9282585909	1.1654188175	-1.1086383558
H	4.7383466444	-0.4640849065	-1.7692907683
C	3.7269035783	0.1117580497	1.5734602028
C	3.1794077373	-0.3919949043	2.9214093999
H	2.2500324485	0.1052764603	3.1961579695
H	2.9964600898	-1.4685365153	2.9198193320
H	3.9175694470	-0.1920895247	3.7045049651
C	5.0726137433	-0.5894189368	1.3102969764

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	5.5656679830	-0.2502738380	0.4024532748
H	5.7522359451	-0.3783805970	2.1422865603
H	4.9725148210	-1.6747070152	1.2527102565
C	3.9411665819	1.6300198727	1.6890848499
H	4.5773895399	1.8410776296	2.5541635633
H	4.4391278458	2.0548578678	0.8181204856
H	2.9998781286	2.1633404672	1.8379604527
N	0.0437750999	-1.2959678702	2.7273700300
C	0.0616738254	-2.0951346612	3.5547043601
C	0.0851709320	-3.1101194721	4.5934892458
H	-0.6724759654	-2.8982142415	5.3500220453
H	1.0628557150	-3.1350486107	5.0782417660
H	-0.1155500847	-4.0927433338	4.1626021759
N	0.0180100330	1.8177214264	1.6512862390
C	0.0178368802	2.8544686479	2.1515375380
C	0.0176409630	4.1664797045	2.7749448960
H	-0.8640478913	4.2868451084	3.4069720943
H	0.0080364942	4.9461733828	2.0109833844
H	0.9087481701	4.2943703759	3.3921487450

***cis*-2^{+2}**

Atom	x (Å)	y (Å)	z (Å)
Rh	0.0197486558	-0.2226177011	0.6728346396
P	-2.4164490645	-0.3541667843	0.3620819899
P	2.4508073434	-0.3277891511	0.3194346958
C	1.2257571592	-3.8449662567	-1.2948968037
C	1.2458646285	-2.6780769815	-0.5285121623
C	0.0210829944	-2.0567254646	-0.2054814477
C	-1.2025889096	-2.6917320122	-0.5056320345
C	-1.1838385362	-3.8585206133	-1.2721476288
C	0.0204946031	-4.4250300698	-1.6741602211
H	2.1608618933	-4.3128885801	-1.5850704447
H	-2.1189728202	-4.3369648468	-1.5446528575

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	0.0200141134	-5.3350654256	-2.2628718986
C	2.5680720922	-2.1366895468	-0.0325373170
C	-2.5212660355	-2.1645782085	0.0142618262
H	2.8321058917	-2.6338336849	0.9059552786
H	3.3829391754	-2.3561568137	-0.7254737777
H	-2.7624888054	-2.6634058932	0.9579770508
H	-3.3464540008	-2.3935965405	-0.6632661630
C	-3.6638301452	0.0078510815	1.7579451295
C	-4.9974005178	-0.7289446138	1.5213479534
H	-4.8779138115	-1.8128349955	1.4769562291
H	-5.6622216613	-0.5208129703	2.3643532888
H	-5.5167057147	-0.4074793962	0.6220912405
C	-3.0558787678	-0.4994042553	3.0775302707
H	-2.1467694751	0.0413894472	3.3415982802
H	-3.7799631558	-0.3415083588	3.8807032045
H	-2.8392953987	-1.5699035264	3.0544858046
C	-3.9067742579	1.5205361922	1.8904220787
H	-4.4481554255	1.9405054742	1.0442801249
H	-4.5170251665	1.7054663743	2.7780651352
H	-2.9755897235	2.0768635704	2.0158265227
C	-2.8580770820	0.5412060513	-1.2745198154
C	-4.3646262669	0.4927750867	-1.5795595116
H	-4.9632224106	1.0773303696	-0.8834322907
H	-4.5293029083	0.9215791167	-2.5720405134
H	-4.7592187909	-0.5242993052	-1.6090076962
C	-2.3817163861	2.0034110646	-1.2026599598
H	-2.6219561085	2.5035455052	-2.1442299305
H	-2.8603298255	2.5724876314	-0.4072217472
H	-1.3000681894	2.0782286184	-1.0661139247
C	-2.1149129825	-0.1621081684	-2.4250898392
H	-1.0330164475	-0.1786952376	-2.2891856865
H	-2.4437468876	-1.1890579336	-2.5830008624
H	-2.3123141975	0.3826775262	-3.3517756003

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	2.8515373354	0.5739294811	-1.3240417563
C	2.0862159200	-0.1312291972	-2.4589148368
H	2.4142209907	-1.1571762289	-2.6245248459
H	1.0074789578	-0.1508286525	-2.2994875194
H	2.2615602846	0.4147806108	-3.3892484585
C	2.3684840452	2.0332665274	-1.2397027543
H	2.8637172764	2.6054265049	-0.4569555997
H	2.5816629869	2.5346744153	-2.1870736598
H	1.2903027203	2.1015561876	-1.0756759792
C	4.3510893075	0.5337655306	-1.6623896236
H	4.4917900001	0.9636869363	-2.6580903388
H	4.9620180440	1.1209584112	-0.9793215112
H	4.7502760805	-0.4811707350	-1.7010445181
C	3.7205868685	0.0458617682	1.6924165257
C	3.1412703197	-0.4651408880	3.0232848261
H	2.2322776475	0.0678641882	3.3032394013
H	2.9337927008	-1.5375366212	3.0049411730
H	3.8782994709	-0.3000030254	3.8132123999
C	5.0552723860	-0.6802865533	1.4313165245
H	5.5551174434	-0.3544769107	0.5226126175
H	5.7340857541	-0.4668928733	2.2619055488
H	4.9437083423	-1.7650908353	1.3888199690
C	3.9547502281	1.5603201896	1.8201637082
H	4.5808187962	1.7496915888	2.6958120726
H	4.4764647620	1.9843316199	0.9637898548
H	3.0222039894	2.1099286537	1.9639014375
N	0.0406016189	-1.2149148144	2.3604755619
C	0.0528844769	-1.8538423591	3.3140745665
C	0.0680523133	-2.6399631178	4.5294222011
H	-0.8052716175	-2.4044651016	5.1412740954
H	0.9691980710	-2.4234734123	5.1069549986
H	0.0520628862	-3.7046740281	4.2877002883
N	0.0184876724	1.8551526290	1.5190143128

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	0.0186412760	2.9194805411	1.9575927979
C	0.0187534391	4.2664838735	2.4972815249
H	0.0042399935	4.9946421165	1.6836984960
H	0.9129128985	4.4340333046	3.1006058282
H	-0.8608538248	4.4248179877	3.1240024137

***trans*-2^{+2}**

Atom	x (Å)	y (Å)	z (Å)
Rh	0.0024247644	-0.1262476287	-0.4505138829
P	2.5449104145	-0.0393231717	-0.1959601356
P	-2.5388422294	-0.0424868597	-0.1927882797
C	-1.2016669140	-0.3565316332	3.6561090566
C	-1.2210299098	-0.3902091092	2.2555695477
C	0.0027840549	-0.2665796839	1.5887570134
C	1.2265722805	-0.3713778994	2.2580700867
C	1.2034837931	-0.3367588481	3.6586884292
C	-0.0002543305	-0.2892104271	4.3515613901
H	-2.1391584746	-0.4127117135	4.2007617929
H	2.1405974929	-0.3783188363	4.2053431749
H	-0.0016880171	-0.2544439096	5.4349705395
C	-2.5081286321	-0.7192335191	1.5303190024
C	2.5191568104	-0.6887591108	1.5378399714
H	-2.5862181658	-1.8082017310	1.4493072526
H	-3.3838047250	-0.3991055020	2.0968218633
H	2.6138220578	-1.7775332403	1.4738540144
H	3.3893312523	-0.3472314959	2.1003943132
C	3.6481389647	-1.2301823186	-1.2343419502
C	4.8749882459	-1.7159806978	-0.4337599317
H	4.5983830821	-2.2627618057	0.4701184926
H	5.4388829376	-2.4122329443	-1.0619018179
H	5.5585840144	-0.9194466975	-0.1520799924
C	2.8207773084	-2.4679969244	-1.6191353558
H	1.9268303327	-2.2174519235	-2.1930204687

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	3.4400165038	-3.1168066106	-2.2444020744
H	2.5321744487	-3.0533863830	-0.7448641311
C	4.1000918157	-0.5403744290	-2.5354158064
H	4.8364565719	0.2430525050	-2.3653176619
H	4.5779338604	-1.2849765686	-3.1780658570
H	3.2669104547	-0.1177434599	-3.1035778973
C	3.3894890785	1.6848556021	-0.0068631259
C	4.8753841604	1.5546461783	0.3929819907
H	5.4996636607	1.1553594909	-0.4043734840
H	5.2533473796	2.5572211224	0.6154108930
H	5.0335436468	0.9565643206	1.2923157415
C	3.3159095877	2.4965340941	-1.3170891323
H	3.5947042988	3.5331240829	-1.1057064072
H	4.0129018183	2.1354918042	-2.0704380948
H	2.3264558465	2.4986793799	-1.7711159382
C	2.6773292732	2.4372642414	1.1395934591
H	1.5987932097	2.5108951240	1.0196897625
H	2.8668664493	1.9816015812	2.1118701044
H	3.0791454821	3.4535944170	1.1875744145
C	-3.3859286863	1.6771173699	0.0283280325
C	-2.6644039287	2.4135811675	1.1790207579
H	-2.8413897119	1.9412869169	2.1455219973
H	-1.5873024272	2.4928930411	1.0489334308
H	-3.0704760909	3.4269369931	1.2481490393
C	-3.3273588191	2.5079821098	-1.2709108565
H	-4.0532645523	2.1738367311	-2.0088488319
H	-3.5740007777	3.5480914147	-1.0386140443
H	-2.3513270087	2.4932896565	-1.7527155609
C	-4.8682115425	1.5383717624	0.4408602422
H	-5.2458819959	2.5368508869	0.6818917513
H	-5.4987910025	1.1500810946	-0.3569320283
H	-5.0174150055	0.9264165014	1.3324787442
C	-3.6373287222	-1.2156639302	-1.2546407609

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-2.8065387240	-2.4436882865	-1.6634439461
H	-1.9102478290	-2.1793178465	-2.2277588714
H	-2.5210787443	-3.0484456130	-0.8016126964
H	-3.4220174535	-3.0789827016	-2.3061875425
C	-4.8637935997	-1.7187584637	-0.4648689966
H	-5.5492934689	-0.9284865513	-0.1702276028
H	-5.4251012519	-2.4054885377	-1.1055742180
H	-4.5860688661	-2.2801712076	0.4298750858
C	-4.0892655810	-0.5018940932	-2.5428489017
H	-4.5663862902	-1.2350975771	-3.1988170149
H	-4.8262259536	0.2778142012	-2.3589830735
H	-3.2556215240	-0.0687804835	-3.1026849502
N	0.0001316272	-2.1361656733	-0.2523344198
C	-0.0043778390	-3.2660228839	-0.0424445465
C	-0.0101402916	-4.6945516827	0.2052555650
H	0.9012891395	-5.1491930802	-0.1897583644
H	-0.8711094218	-5.1578863603	-0.2820230414
H	-0.0648210653	-4.8877900624	1.2791529815
N	-0.0038821524	1.8872844634	-0.7806301620
C	-0.0195225784	2.9986473052	-1.0754579465
C	-0.0448483497	4.4058686096	-1.4203063161
H	0.9730530071	4.7932538707	-1.4960178128
H	-0.5813082943	4.9655965065	-0.6504417246
H	-0.5505076229	4.5493126785	-2.3777136083

***trans*-2^{+}**

Atom	x (Å)	y (Å)	z (Å)
Rh	0.0052020634	0.2276159923	-0.5154853273
P	-2.7643061389	0.0204282202	-0.2414278076
P	2.7657621377	0.0221927241	-0.2402034737
C	1.2028250596	-0.1691986731	3.5595367402
C	1.2238581192	0.0959005368	2.1845088737
C	0.0027033542	0.1201223454	1.4915273436

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-1.2189800735	0.0907748734	2.1836454909
C	-1.1969695991	-0.1747488559	3.5587822947
C	0.0030945178	-0.3377089038	4.2380699580
H	2.1404097944	-0.2209466239	4.1057332537
H	-2.1346498658	-0.2308229083	4.1045960030
H	0.0031435375	-0.5535353029	5.3008753020
C	2.5438202540	0.4958805234	1.5482443457
C	-2.5408228965	0.4870527038	1.5487362701
H	2.5943280022	1.5893343355	1.5681490043
H	3.3814851084	0.1526009275	2.1591815035
H	-2.5953988388	1.5801636071	1.5728855589
H	-3.3768722986	0.1386132301	2.1591152297
C	-3.9960353083	1.3495738721	-0.8891136914
C	-5.1366219518	1.7082304050	0.0800559238
H	-4.7678629049	2.0682533547	1.0427574873
H	-5.7345065490	2.5178085197	-0.3520794340
H	-5.8150842536	0.8808813832	0.2722638538
C	-3.1739191765	2.6263566750	-1.1437066254
H	-2.3557941291	2.4552314061	-1.8453928848
H	-3.8257971657	3.3956707814	-1.5695596863
H	-2.7561185740	3.0341174830	-0.2206358531
C	-4.5756723607	0.8958623091	-2.2400597731
H	-5.2778253608	0.0681693363	-2.1427790460
H	-5.1245486173	1.7242529761	-2.6986532467
H	-3.7941061374	0.5978927528	-2.9441383149
C	-3.6497510888	-1.6859148301	-0.1363267250
C	-5.1111379283	-1.6384245764	0.3395670430
H	-5.7785327002	-1.1609071126	-0.3772764298
H	-5.4756721967	-2.6621725653	0.4762865300
H	-5.2244167465	-1.1332455487	1.3010017503
C	-3.5930580299	-2.3538827055	-1.5226767134
H	-3.9804906707	-3.3760170253	-1.4564579791
H	-4.1962421438	-1.8328728522	-2.2655246147

Continued on Next Page...

Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-2.5744114946	-2.4033655910	-1.9094045746
C	-2.8651713843	-2.5496865146	0.8721793142
H	-1.7937262154	-2.5685554741	0.6812061553
H	-3.0048073567	-2.2121616752	1.8999192169
H	-3.2342823018	-3.5798408320	0.8236454828
C	3.6482928771	-1.6843581815	-0.1274145740
C	2.8598502105	-2.5435594609	0.8819958269
H	2.9962634388	-2.2019971400	1.9086070527
H	1.7889856520	-2.5628172370	0.6876325196
H	3.2283307840	-3.5739704878	0.8387218507
C	3.5960027147	-2.3575002233	-1.5113746611
H	4.2037875354	-1.8405744590	-2.2532538575
H	3.9807594273	-3.3802016488	-1.4399729042
H	2.5790283474	-2.4062494327	-1.9025124720
C	5.1079621122	-1.6346369315	0.3534870539
H	5.4722542943	-2.6575657289	0.4963261947
H	5.7771519613	-1.1601216999	-0.3637075151
H	5.2180701728	-1.1247572044	1.3128457488
C	3.9977416831	1.3474990095	-0.8961148009
C	3.1747224061	2.6220381182	-1.1589492042
H	2.3564552409	2.4463607861	-1.8594129019
H	2.7572231621	3.0355709076	-0.2384399512
H	3.8263791242	3.3890173297	-1.5899037782
C	5.1370122841	1.7131996727	0.0717325946
H	5.8167349562	0.8879899594	0.2696672152
H	5.7336018770	2.5213119602	-0.3648327337
H	4.7667564174	2.0786149878	1.0318176660
C	4.5787364380	0.8859644678	-2.2438885162
H	5.1275273640	1.7120829824	-2.7066119105
H	5.2811416632	0.0592231105	-2.1411867179
H	3.7982117965	0.5835607575	-2.9472765863
N	0.0035081841	2.2699456579	-0.2468117334
C	0.0017275083	3.4093674329	-0.0884005074

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-0.0025487929	4.8469558104	0.1010826723
H	-0.8866747956	5.2871820663	-0.3642816814
H	0.8873389018	5.2910386320	-0.3493561144
H	-0.0120001428	5.0862174910	1.1662363596
N	0.0024380577	-1.8568570251	-0.9533554267
C	0.0021242403	-2.9167774735	-1.4019976496
C	0.0020554302	-4.2565443125	-1.9570278412
H	-0.8887841896	-4.7984204453	-1.6342026793
H	0.8861781318	-4.8025733057	-1.6230085099
H	0.0090318094	-4.2125894585	-3.0478222062

$[(\mathrm{PCP})\mathrm{Rh}^{\mathrm{III}}(\mathrm{MeCN})_3]^{+2}$

Atom	x (Å)	y (Å)	z (Å)
Rh	0.0016445699	0.2479008158	0.0511731430
P	2.5226469512	-0.0349387650	-0.0796104829
P	-2.5194776209	-0.0312707108	-0.0793025291
C	-1.2006681415	-2.8926215874	-2.6735786029
C	-1.2148455931	-1.7753456745	-1.8316440501
C	0.0003022106	-1.2931641655	-1.3179215656
C	1.2147792850	-1.7744131133	-1.8341608058
C	1.1998080529	-2.8915114411	-2.6763237444
C	-0.0006143584	-3.4753624191	-3.0598591805
H	-2.1369789858	-3.2915848834	-3.0509796378
H	2.1356003535	-3.2897767985	-3.0558377214
H	-0.0009779940	-4.3491800695	-3.7009593705
C	-2.5089291388	-1.0138131793	-1.6434658002
C	2.5086987804	-1.0124187725	-1.6471749364
H	-2.6103101853	-0.3010640583	-2.4681963732
H	-3.3834470953	-1.6634254482	-1.7058537567
H	2.6071733471	-0.2967183535	-2.4697114588
H	3.3834457023	-1.6612435501	-1.7142446080
C	3.6330625675	1.5058209541	-0.3854957923
C	4.8779186373	1.1630002985	-1.2286174258

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	4.6229951945	0.7483348899	-2.2054207347
H	5.4311627382	2.0878649784	-1.4158129493
H	5.5654156990	0.4786361308	-0.7413230474
C	2.8285319520	2.5591739678	-1.1625010524
H	1.9238794984	2.8675801769	-0.6396380297
H	3.4544173975	3.4451630622	-1.2967388146
H	2.5612339070	2.2099970727	-2.1603949236
C	4.0539946973	2.1296567790	0.9566896534
H	4.7839021650	1.5280728890	1.4943493936
H	4.5262768928	3.0968094667	0.7659690091
H	3.2024771133	2.3094316161	1.6171781935
C	3.3686783842	-1.2195634938	1.1797275417
C	4.8720044876	-1.4066517746	0.8906260171
H	5.4667897971	-0.5224949619	1.1093034304
H	5.2447865979	-2.2025300088	1.5418856737
H	5.0785393440	-1.7220949636	-0.1329610757
C	3.2224693585	-0.6904575151	2.6204847615
H	3.5070377522	-1.4789304337	3.3231163104
H	3.8839151757	0.1501267833	2.8179802486
H	2.2129327859	-0.3678666352	2.8651270652
C	2.7196294114	-2.6134766933	1.0278160104
H	1.6339860916	-2.6087706894	1.0404512077
H	3.0254357625	-3.1033246485	0.1036775892
H	3.0657661439	-3.2520160475	1.8452800027
C	-3.3656343891	-1.2090643711	1.1857257669
C	-2.7203703883	-2.6051688148	1.0360153742
H	-3.0349719016	-3.0986962478	0.1168317242
H	-1.6345854913	-2.6034383016	1.0386484099
H	-3.0624508137	-3.2383607317	1.8592447036
C	-3.2148485725	-0.6719163580	2.6239394599
H	-3.9014680510	0.1468536455	2.8277209118
H	-3.4610690928	-1.4667422591	3.3335697199
H	-2.2134992885	-0.3137561679	2.8524409267

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
C	-4.8699284252	-1.3963506505	0.9013019234
H	-5.2436899629	-2.1825287266	1.5636758611
H	-5.4623377139	-0.5080487006	1.1088913203
H	-5.0786887244	-1.7249814380	-0.1178040034
C	-3.6287313790	1.5084947669	-0.3885564633
C	-2.8284670640	2.5561498730	-1.1774855362
H	-1.9197973242	2.8661389044	-0.6626354138
H	-2.5686703219	2.2008872594	-2.1751972229
H	-3.4540603883	3.4422111655	-1.3122420799
C	-4.8790687442	1.1601421274	-1.2213704066
H	-5.5623337868	0.4777539869	-0.7253571117
H	-5.4347151438	2.0832146873	-1.4099484067
H	-4.6303135362	0.7403505060	-2.1975525859
C	-4.0404569743	2.1405507789	0.9525467501
H	-4.5177104745	3.1047269836	0.7589272131
H	-4.7636821833	1.5401373031	1.5004595981
H	-3.1840191687	2.3279400065	1.6044782530
N	0.0034576635	1.3353919238	-1.6608798722
C	0.0037995513	1.8418820785	-2.6909732828
C	0.0035245929	2.4910462839	-3.9857463780
H	0.8928595645	3.1148250221	-4.0964612276
H	-0.8798779405	3.1240856487	-4.0912823583
H	-0.0027239733	1.7426341191	-4.7807873969
N	-0.0017497536	-0.9128311668	1.7276610610
C	-0.0101345832	-1.5098738295	2.7081120326
C	-0.0260137486	-2.2836561315	3.9318483265
H	0.9868725250	-2.5954461247	4.1934607894
H	-0.6446915659	-3.1740110905	3.8009239381
H	-0.4340378053	-1.6892154385	4.7518782067
N	0.0025674813	2.0433095063	1.4608054024
C	-0.0002092417	2.9541464593	2.1643201642
C	-0.0047956572	4.1062791694	3.0485107223
H	0.9471604962	4.1824848719	3.5770748263

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Table A.1 – Continued

Atom	x (Å)	y (Å)	z (Å)
H	-0.8064989029	4.0164271167	3.7837731715
H	-0.1591419664	5.0213094505	2.4736943379