Supporting Information

On the Role of Disproportionation Energy in Kumada Catalyst-Transfer Polycondensation

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Table 1. Absolute disproportionation energies in kcal mol^{-1} computed with the B3LYP functional and basis sets described in the Theoretical Methods section. Th = thiophene; MeTh = 3-methylthiophene; HexTh = 3-hexylthiophene.

Complex	E_{disp}
Ni(dhpe)ThBr	2.2
Ni(dhpp)ThBr	8.4
Ni(dhpb)ThBr	–2.1
Ni(dhpf)ThBr	3.2
Ni(dmpe)ThBr	2.3
Ni(depe)ThBr	–4.5
Ni(dppe)ThBr	1.1
Ni(dppp)ThBr	1.6
Ni(dhpe)MeThBr	2.6
Ni(dhpp)MeThBr	8.6
Ni(dhpb)MeThBr	–2.4
Ni(dhpf)MeThBr	3.7
Ni(dhpe)HexThBr	4.6
Ni(dhpp)HexThBr	9.4
Ni(dhpb)HexThBr	–2.7

Table 2. Absolute disproportionation energies in kcal mol^{-1} computed with the specified functional and basis sets described in the Theoretical Methods section. Th = thiophene.

	B3LYP	M06	B97	PBE
Ni(dhpe)ThBr	2.2	2.2	1.2	1.9
Ni(dhpp)ThBr	8.4	8.6	8.4	7.6
Ni(dhbp)ThBr	–2.1	–2.2	–2.8	1.0

Table 3. Comparison of disproportionation energy with several methods showing B3LYP has little deviation from CCSD. A simplified model reaction was computed:

$2(dhpe)NiBrCH_3 \rightarrow (dhpe)NiBr_2 + (dhpe)Ni(CH_3)_2$

	Total Electronic Energy with ZPE (hartree)				
Method[a]	(dhpe)NiBrCH$_3$	(dhpe)NiBr$_2$	(dhpe)Ni(CH$_3$)$_2$	E_{disp} (kcal mol^{-1})	Deviation from CCSD (kcal mol^{-1})
B3LYP	–2325.3446	–2298.8973	–2351.7768	9.5	0.0
B97	–2325.0291	–2298.5913	–2351.4521	9.3	0.2
M06	–2325.0384	–2298.6015	–2351.4613	8.8	0.7
PBE	–2320.9333	–2294.5967	–2347.2553	9.2	0.3
MP2	–2322.7828	–2296.2358	–2349.3096	12.7	–3.2
CCSD	–2321.2439	–2294.8815	–2347.5912	9.5	–

[a]In all cases the same basis set described in the text was used.

Table 4. Out-of-plane angles of active-ligand atoms in initiating species, where the plane is defined by P–Ni–P. Th = thiophene.

Complex	Br	Thiophene carbon
Ni(dhpe)ThBr	4.1°	–0.3°
Ni(dhpp)ThBr	3.2°	–2.0°
Ni(dhpb)ThBr	3.1°	–4.6°
Ni(dhpf)ThBr	4.1°	–3.9°
Ni(dmpe)ThBr	0.6°	–0.2°
Ni(depe)ThBr	12.1°	–11.0°
Ni(dppe)ThBr	2.7°	–2.2°
Ni(dppp)ThBr	6.0°	–4.4°

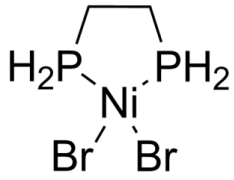
Table 5. Total electronic energies computed at the B3LYP level with basis sets described in the Theoretical Methods section. Th = thiophene; MeTh = 3-methylthiophene.

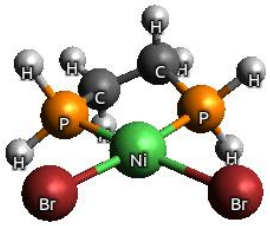
Complex	Electronic Energy (hartree)	ZPE (kcal mol^{-1})	Electronic Energy with ZPE (hartree)
Ni(dhpe)BrTh	–5398.7340	95.8	–5398.5814
Ni(dhpe)Br_2	–7420.4924	61.4	–7420.3944
Ni(dhpe)Th_2	–3376.9725	130.3	–3376.7649
Ni(dhpp)BrTh	–5438.0592	114.1	–5437.8774
Ni(dhpp)Br_2	–7459.8090	79.4	–7459.6824
Ni(dhpp)Th_2	–3416.2957	148.5	–3416.0590
Ni(dhpb)BrTh	–5477.3681	132.0	–5477.1578
Ni(dhpb)Br_2	–7499.1293	97.6	–7498.9737
Ni(dhpb)Th_2	–3455.6101	166.2	–3455.3452
Ni(dhpf)BrTh	–6969.6122	154.0	–6969.3667
Ni(dhpf)Br_2	–8991.3682	119.5	–8991.1777
Ni(dhpf)Th_2	–4947.8508	188.3	–4947.5507
Ni(dmpe)BrTh	–5556.0660	168.1	–5555.7982
Ni(dmpe)Br_2	–7577.8287	133.6	–7577.6157
Ni(dmpe)Th_2	–3534.2996	202.4	–3533.9770
Ni(depe)BrTh	–5713.3246	240.5	–5712.9414
Ni(depe)Br_2	–7735.0912	206.0	–7734.7629
Ni(depe)Th_2	–3691.5612	272.4	–3691.1271
Ni(dppe)BrTh	–6323.0510	301.9	–6322.5698
Ni(dppe)Br_2	–8344.8122	267.5	–8344.3859
Ni(dppe)Th_2	–4301.2883	336.6	–4300.7519
Ni(dppp)BrTh	–6362.3608	320.0	–6361.8509
Ni(dppp)Br_2	–8384.1219	285.6	–8383.6668
Ni(dppp)Th_2	–4340.5973	354.5	–4340.0323
Ni(dhpe)MeThBr	–5438.0579	113.2	–5437.8775
Ni(dhpe)$MeTh_2$	–3455.6193	164.9	–3455.3565
Ni(dhpp)MeThBr	–5477.3816	131.3	–5477.1723
Ni(dhpp)$MeTh_2$	–3494.9402	183.0	–3494.6486
Ni(dhpb)MeThBr	–5516.6903	149.1	–5516.4527
Ni(dhpb)$MeTh_2$	–3534.2557	200.9	–3533.9356
Ni(dhpf)MeThBr	–7008.9345	171.3	–7008.6615
Ni(dhpf)$MeTh_2$	–5026.4948	222.9	–5026.1395

Table 6. Cartesian Coordinates (Å) of Stationary Points

$NiBr_2dhpe$

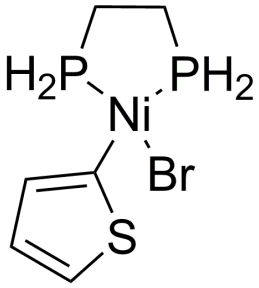
Ni	0.000000	0.000000	0.002078
Br	0.039180	1.812747	1.538584
Br	–0.039180	–1.812747	1.538584
P	–0.045431	1.516646	–1.554488
H	1.136881	2.262185	–1.736803
H	–0.997419	2.550049	–1.513406
P	0.045431	–1.516646	–1.554488
H	–1.136881	–2.262185	–1.736803
H	0.997419	–2.550049	–1.513406
C	–0.334298	0.695604	–3.208254
C	0.334298	–0.695604	–3.208254
H	0.027847	1.313866	–4.038034
H	–1.421811	0.594487	–3.321462
H	–0.027847	–1.313866	–4.038034
H	1.421811	–0.594487	–3.321462

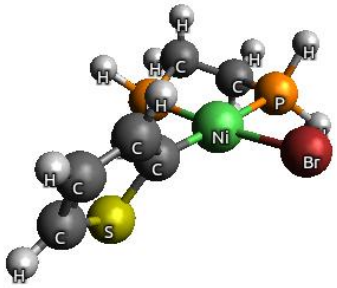




NiBrThdhpe

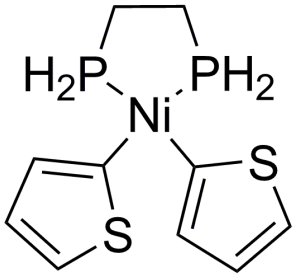
Ni	0.366597	–0.211688	–0.221072
P	0.625293	1.851009	0.368392
P	2.601635	–0.401626	–0.200156
Br	0.201116	–2.535612	–0.705893
C	3.345139	1.301914	0.006012
C	2.398006	2.157971	0.876960
H	3.315892	–0.949323	–1.283823
H	3.181124	–1.142404	0.852579
H	–0.124261	2.380497	1.435855
H	0.378795	2.843269	–0.605320
H	2.652656	3.222763	0.818728
H	2.477740	1.857535	1.930304
H	4.352881	1.267992	0.435415
H	3.429109	1.735510	–0.999335
C	–3.876980	0.882420	–0.736979
C	–3.822614	0.024954	0.336284
C	–2.488139	–0.413187	0.637761
C	–1.522250	0.095940	–0.208860
S	–2.288983	1.147295	–1.380706
H	–4.747532	1.337591	–1.197680
H	–4.704501	–0.299138	0.884737
H	–2.257556	–1.117476	1.433520

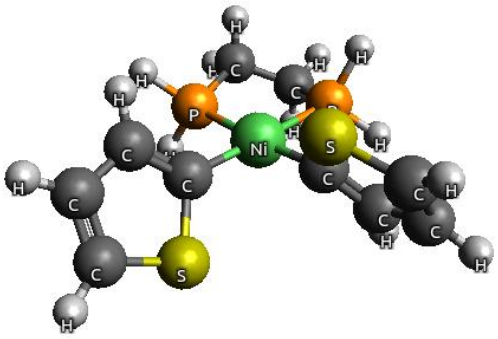




NiTh$_2$dhpe

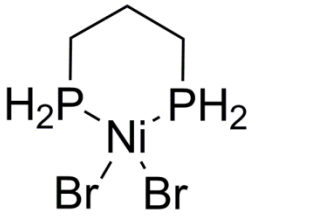
Ni	0.392784	0.173879	–0.064408
P	1.876609	1.870618	–0.018234
P	2.156536	–1.134866	–0.565122
C	3.658294	–0.076260	–0.958659
C	3.630534	1.199316	–0.093057
H	2.145303	–2.067460	–1.624257
H	2.635608	–1.986681	0.456460
H	1.944453	2.800256	1.041459
H	1.846476	2.786996	–1.094448
H	4.343211	1.944433	–0.457839
H	3.908749	0.959285	0.939605
H	4.596046	–0.624318	–0.830227
H	3.576344	0.187012	–2.019507
C	–3.141362	2.778015	0.135438
C	–2.432665	3.027517	1.277364
C	–1.242994	2.235092	1.375451
C	–1.043926	1.368705	0.319657
S	–2.365264	1.543074	–0.812581
H	–4.062381	3.237499	–0.197538
H	–2.738296	3.751033	2.026632
H	–0.566755	2.300003	2.223145
C	–0.770137	–1.338207	–0.072655
C	–1.028217	–2.276015	–1.052238
C	–1.920808	–3.322853	–0.652298
C	–2.337546	–3.195481	0.643346
S	–1.659272	–1.768609	1.370632
H	–0.606460	–2.218624	–2.051712
H	–2.231009	–4.132553	–1.305311
H	–2.997487	–3.844605	1.203179

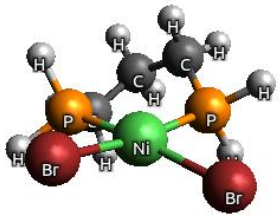




NiBr$_2$dhpp

Ni	0.179032	–0.000515	0.000751
Br	1.750844	1.775279	–0.167109
Br	1.753200	–1.774049	0.167467
P	–1.329109	1.579422	0.146866
H	–1.640288	2.295996	–1.028512
H	–1.010255	2.637983	1.012938
P	–1.328473	–1.581105	–0.144178
H	–1.642095	–2.294433	1.032585
H	–1.008303	–2.642250	–1.006582
C	–2.974565	1.047488	0.817562
C	–2.972585	–1.050543	–0.819253
C	–3.771461	–0.000862	–0.002579
H	–3.604680	1.928978	0.986742
H	–2.733973	0.642021	1.810383

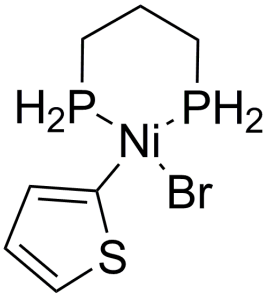


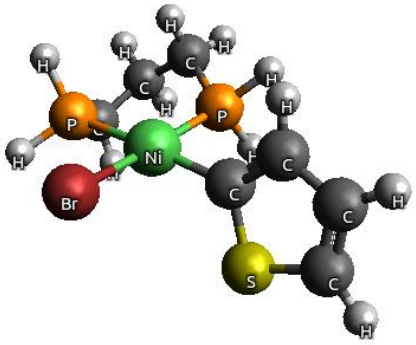


H	–2.729852	–0.646734	–1.812208
H	–3.602117	–1.932461	–0.988307
H	–4.429081	0.524732	–0.705967
H	–4.432798	–0.525459	0.698053

NiBrThdhpp

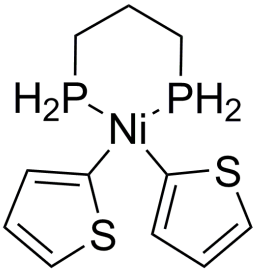
Ni	0.088815	–0.254509	–0.179773
P	0.678773	1.837053	–0.372946
P	2.249791	–0.921662	0.177205
Br	–0.643088	–2.542915	–0.188123
C	2.491099	2.168763	–0.668080
H	3.116787	–1.249331	–0.893695
H	2.435838	–2.070521	0.968745
H	0.334815	2.709215	0.682847
H	0.103537	2.529991	–1.455000
H	2.700788	1.646331	–1.609800
H	2.645304	3.234394	–0.864199
C	–4.008306	1.183297	0.393282
C	–3.760957	1.326728	–0.942895
C	–2.436271	0.922908	–1.310329
C	–1.682181	0.451168	–0.260225
S	–2.620394	0.529270	1.214722
H	–4.914865	1.408183	0.938756
H	–4.492540	1.704811	–1.649492
H	–2.070046	0.961594	–2.331822
C	3.484220	1.703132	0.422620
C	3.222010	0.351330	1.136838
H	2.612566	0.513904	2.033544
H	4.171739	–0.068806	1.478616
H	4.472598	1.664914	–0.048227
H	3.550266	2.476801	1.195432



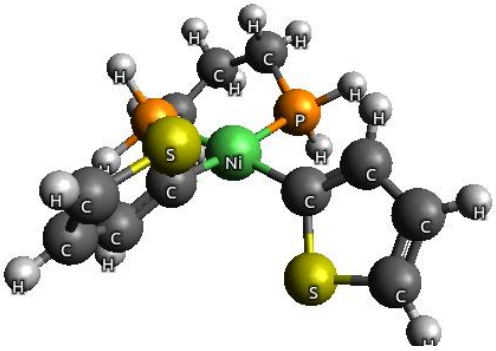


NiTh$_2$dppp

Ni	0.282185	0.008842	–0.020619
P	1.810631	1.628677	–0.414175
P	1.932861	–1.508441	0.275186
C	3.580941	–0.805446	0.804923
C	4.296178	0.122226	–0.207372
H	2.284791	–2.388598	–0.776202
H	1.720315	–2.469238	1.285320
H	2.222756	2.491839	0.630309
H	1.457600	2.611560	–1.362111
H	4.927694	–0.489592	–0.861124
H	4.982813	0.755312	0.365623

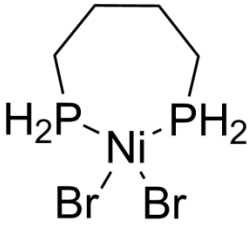


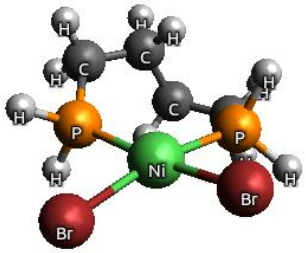
H	3.339556	–0.244630	1.716295
H	4.263597	–1.605963	1.104204
C	–3.002707	2.844249	0.650874
C	–2.567263	3.090896	–0.621122
C	–1.493821	2.228809	–1.016878
C	–1.109184	1.314381	–0.057838
S	–2.114599	1.527162	1.359124
H	–3.782119	3.350391	1.204550
H	–2.988732	3.860556	–1.260092
H	–1.035900	2.282708	–2.000576
C	–1.004187	–1.396427	0.087966
C	–1.270682	–2.333938	1.064896
C	–2.293102	–3.277031	0.721891
C	–2.806876	–3.069486	–0.527592
S	–2.057211	–1.691416	–1.278808
H	–0.763445	–2.348248	2.025485
H	–2.623359	–4.073774	1.380980
H	–3.571890	–3.635246	–1.042287
C	3.431735	1.026256	–1.121963
H	3.127302	0.468176	–2.015683
H	4.035567	1.868518	–1.471437



$NiBr_2dhpb$

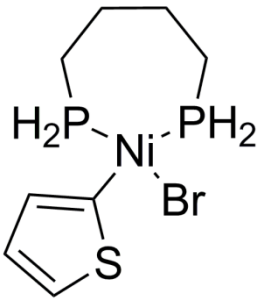
Ni	0.286922	–0.030666	0.046533
P	–1.095651	1.749862	0.194523
P	–1.186890	–1.735426	–0.142035
Br	1.897591	–1.738339	–0.511475
C	–3.602816	–0.341858	0.596208
H	–0.716387	–2.923134	0.440229
H	–1.324700	–2.164685	–1.477413
H	–0.531857	2.926651	–0.323250
H	–1.293654	2.151256	1.531402
H	–4.645727	–0.471633	0.905462
H	–3.122859	0.198859	1.421534
Br	1.973497	1.576739	0.674598
C	–2.822547	1.847733	–0.537849
C	–2.959387	–1.730711	0.482394
C	–3.530523	0.496753	–0.703971
H	–3.410441	2.521903	0.094511
H	–2.717150	2.337435	–1.511495
H	–2.944364	–2.217680	1.462856
H	–3.541926	–2.376481	–0.183580
H	–4.538138	0.682921	–1.091450
H	–3.018361	–0.070392	–1.491315

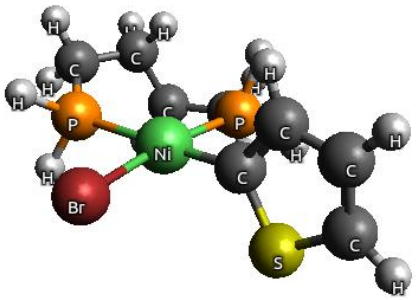




NiBrThdhpb

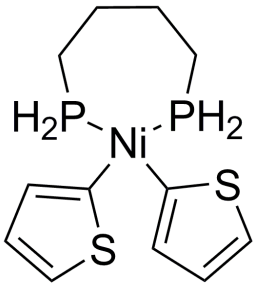
Ni	–0.046510	–0.211919	0.061439
P	–0.621608	1.897694	0.101331
P	–2.066757	–1.285691	0.020630
Br	0.884261	–2.405843	–0.105612
C	–3.776020	0.951352	0.541754
H	–2.064048	–2.486110	0.752213
H	–2.331806	–1.824820	–1.256340
H	0.324896	2.801852	–0.409723
H	–0.681666	2.380089	1.428110
H	–4.792176	1.267390	0.810073
H	–3.132522	1.303131	1.360809
C	4.004111	1.506492	–0.145539
C	3.656263	1.485931	1.183138
C	2.338399	0.951406	1.401797
C	1.697790	0.548265	0.243900
S	2.728837	0.852030	–1.126037
H	4.936069	1.833927	–0.594793
H	4.312690	1.827586	1.980396
H	1.899109	0.842952	2.392027
C	–2.178055	2.603087	–0.662975
C	–3.736089	–0.587015	0.511494
C	–3.347694	1.613097	–0.793233
H	–2.473086	3.480878	–0.072142
H	–1.892095	2.969174	–1.657649
H	–3.973668	–0.984702	1.506216
H	–4.494535	–0.978324	–0.178510
H	–4.197297	2.145614	–1.239458
H	–3.069203	0.840332	–1.523887



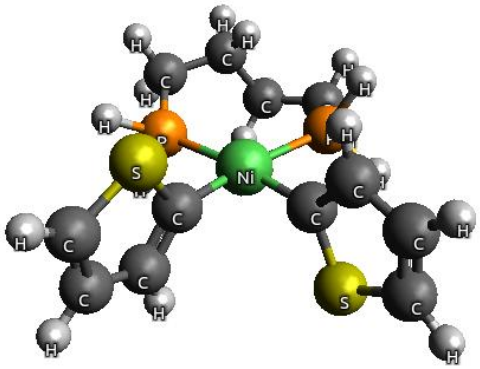


NiTh$_2$dhpb

Ni	0.202357	0.123135	0.004743
P	1.553759	1.943321	–0.264080
P	1.657959	–1.616048	0.289267
C	–1.135072	–1.229710	0.156255
C	4.061306	–0.277130	–0.457753
H	1.242538	–2.790705	–0.368048
H	1.601978	–2.104394	1.614115
H	1.022762	3.131780	0.273867
H	1.585309	2.341834	–1.620296
H	5.102819	–0.387282	–0.781725
H	3.515572	0.076362	–1.342355
C	–3.012046	3.116849	0.257468
C	–2.847533	2.849947	–1.071291
C	–1.836133	1.864072	–1.324408

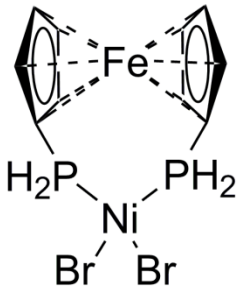


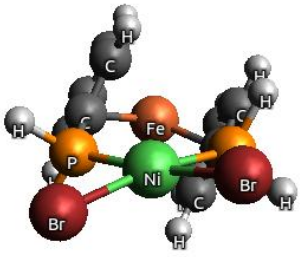
C	–1.223075	1.375428	–0.192698
S	–1.922138	2.148476	1.215421
H	–3.701647	3.803928	0.728760
H	–3.427275	3.330413	–1.853084
H	–1.590879	1.517547	–2.323583
C	3.363678	2.112193	0.240907
C	3.511945	–1.656088	–0.065901
C	3.972530	0.772511	0.676948
H	3.931872	2.549143	–0.586808
H	3.401405	2.829596	1.066857
H	3.674410	–2.373471	–0.876399
H	4.036008	–2.044888	0.813361
H	4.969650	0.952814	1.095282
H	3.371885	0.376991	1.506468
C	–1.727571	–1.780568	1.270668
C	–2.669230	–2.824844	0.986250
C	–2.800850	–3.074945	–0.349587
S	–1.766586	–2.018757	–1.274725
H	–1.516014	–1.439644	2.279512
H	–3.224577	–3.358173	1.751274
H	–3.437463	–3.797272	–0.842282



$NiBr_2dhpf$

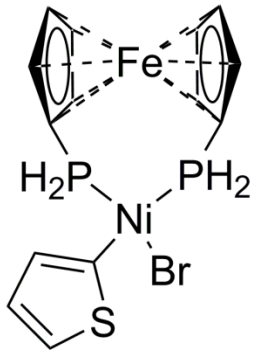
Ni	1.444473	–0.027492	–0.011454
Br	3.084058	1.614980	0.535558
Br	3.036580	–1.711643	–0.569548
P	0.064217	1.691081	0.217342
P	0.021147	–1.714578	–0.210718
C	–4.051373	–1.729135	0.211430
C	–2.867802	–1.967220	–0.552405
C	–1.730988	–1.620529	0.259967
C	–2.233090	–1.181421	1.536574
C	–3.660153	–1.246851	1.499789
H	–5.069410	–1.867841	–0.136362
H	–2.829515	–2.325344	–1.576132
H	–1.632319	–0.848626	2.377281
H	–4.328663	–0.956575	2.303131
Fe	–2.918793	0.025501	0.012703
C	–1.692935	1.641735	–0.240916
C	–2.815579	2.015260	0.579301
C	–4.009530	1.807277	–0.177128
C	–3.638557	1.317287	–1.468628
C	–2.213831	1.216821	–1.514798
H	–2.761773	2.370864	1.603215
H	–5.021613	1.969761	0.177595
H	–4.319188	1.044836	–2.268041
H	–1.626764	0.869926	–2.359462
H	0.503999	2.844208	–0.455240



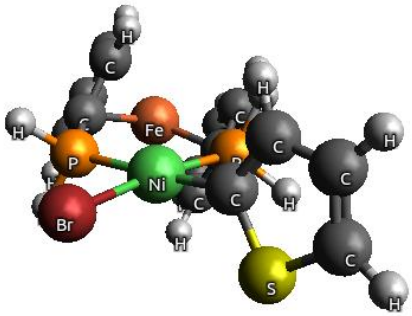


H	–0.018818	2.180295	1.534365
H	0.440035	–2.867673	0.475152
H	–0.083332	–2.220786	–1.519649

NiBrThdhpf



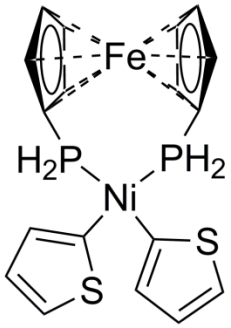
Ni	1.246292	0.414488	–0.084525
Br	2.697104	2.301150	0.104311
P	–0.428142	1.950203	–0.014552
P	0.135796	–1.458056	–0.109114
C	4.702577	–2.310598	0.117398
C	4.334535	–2.249976	–1.204844
C	3.195226	–1.399126	–1.421382
C	2.715426	–0.797834	–0.270823
S	3.671597	–1.310674	1.091530
H	5.526265	–2.857825	0.564368
H	4.854780	–2.782476	–1.997875
H	2.769762	–1.218362	–2.407335
C	–3.870991	–2.105002	0.464265
C	–2.684229	–2.210758	–0.324479
C	–1.602694	–1.604502	0.406133
C	–2.139082	–1.137798	1.658374
C	–3.534198	–1.445770	1.688212
H	–4.859115	–2.444899	0.173033
H	–2.612058	–2.652267	–1.313327
H	–1.581593	–0.629368	2.438845
H	–4.220989	–1.198978	2.490781
Fe	–3.068966	–0.210593	0.065589
C	–2.172286	1.582625	–0.384607
C	–3.320237	1.814370	0.449704
C	–4.475494	1.314698	–0.227086
C	–4.056687	0.782594	–1.486904
C	–2.640407	0.945781	–1.588592
H	–3.304825	2.268559	1.435216
H	–5.489142	1.318704	0.159165
H	–4.696573	0.314140	–2.226994
H	–2.021381	0.632201	–2.423627
H	–0.200512	3.093584	–0.804702
H	–0.560966	2.571164	1.244244
H	0.728286	–2.508197	0.616632
H	0.080456	–2.056390	–1.384885

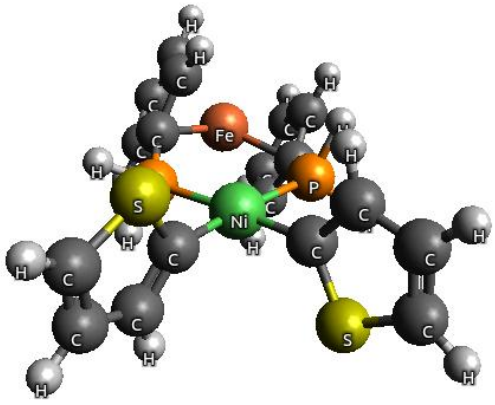


NiTh$_2$dhpf

Ni	1.073243	–0.083637	0.022004
P	–0.320354	1.645333	0.304257

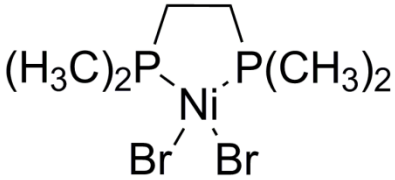
P	–0.375101	–1.772560	–0.220662
C	4.112288	–3.274975	0.190170
C	3.880498	–3.041982	–1.143421
C	2.917414	–1.995853	–1.364510
C	2.419271	–1.424852	–0.205411
S	3.160086	–2.201684	1.169507
H	4.788363	–3.991846	0.644662
H	4.378682	–3.587494	–1.942068
H	2.626460	–1.662499	–2.359592
C	4.201750	3.012609	–0.249182
C	4.009029	2.785649	1.091626
C	3.021759	1.770018	1.346172
C	2.465800	1.216351	0.205101
S	3.182132	1.971295	–1.194767
H	4.883731	3.708348	–0.727081
H	4.551606	3.314335	1.872478
H	2.755623	1.444598	2.350770
C	–4.458084	–1.764188	0.203314
C	–3.281130	–1.997430	–0.573408
C	–2.134896	–1.706539	0.244529
C	–2.623928	–1.301205	1.536970
C	–4.052376	–1.338810	1.507383
H	–5.480176	–1.870689	–0.144302
H	–3.253842	–2.315687	–1.610598
H	–2.011991	–1.008197	2.384387
H	–4.711707	–1.067369	2.324823
Fe	–3.305970	–0.021229	0.066998
C	–2.088606	1.629120	–0.131121
C	–3.212998	1.954280	0.704030
C	–4.408143	1.754796	–0.054055
C	–4.035303	1.316019	–1.363528
C	–2.609172	1.236250	–1.414991
H	–3.160202	2.273421	1.739955
H	–5.421161	1.891601	0.309110
H	–4.714885	1.063165	–2.170287
H	–2.018877	0.923653	–2.270687
H	0.103464	2.861864	–0.269320
H	–0.396792	2.063052	1.651432
H	0.025636	–2.997201	0.352315
H	–0.486952	–2.194984	–1.563767



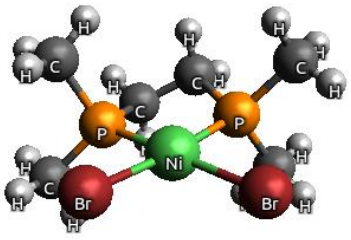


$NiBr_2dmpe$

Ni	–0.000111	–0.274516	–0.000698
Br	–1.782290	–1.869226	0.119099
Br	1.785399	–1.865640	–0.120805
P	–1.537106	1.288887	–0.033987
C	–2.442180	1.513331	1.546658
C	–2.846976	1.224746	–1.312558

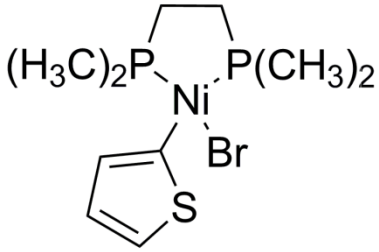


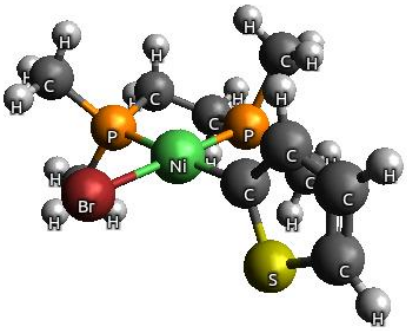
P	1.534117	1.291704	0.033417
C	2.439133	1.518312	–1.546954
C	2.843827	1.229767	1.312254
C	–0.694008	2.924070	–0.338579
C	0.687975	2.925277	0.338274
H	–1.315760	3.760275	0.008037
H	–0.585778	3.030150	–1.426782
H	1.308177	3.762683	–0.008215
H	0.579531	3.031023	1.426489
H	1.733525	1.734265	–2.357202
H	3.165707	2.337507	–1.470123
H	2.956248	0.583078	–1.783984
H	–2.389271	1.129982	–2.303555
H	–3.462577	2.133220	–1.279578
H	–3.467709	0.341493	–1.137256
H	3.457807	2.139342	1.279421
H	2.386110	1.134165	2.303165
H	3.466156	0.347628	1.137014
H	–3.171001	2.330539	1.469954
H	–2.956712	0.576756	1.784017
H	–1.736872	1.731354	2.356619



NiBrThdmpe

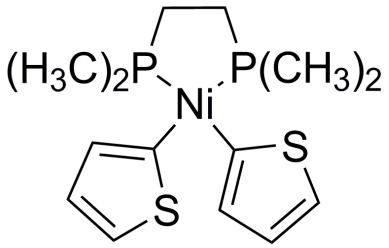
Ni	–0.105814	–0.148260	0.055805
P	–0.000448	2.017224	–0.001527
P	–2.340281	0.010169	–0.122189
Br	–0.297183	–2.540562	0.088636
C	–2.797221	1.813134	0.031934
C	–1.659365	2.681442	–0.542459
C	–3.429576	–0.841380	1.082085
C	–3.003968	–0.504586	–1.756352
C	1.189281	2.856821	–1.113032
C	0.295629	2.810194	1.630185
H	–1.771689	3.735986	–0.255696
H	–1.669865	2.642743	–1.640652
H	–3.754438	2.034095	–0.458959
H	–2.928345	2.021063	1.102915
C	4.289111	–0.363199	–0.305538
C	4.036218	–0.096796	1.018824
C	2.630869	0.031557	1.297783
C	1.808633	–0.157276	0.199414
S	2.803761	–0.481620	–1.196297
H	5.245780	–0.525378	–0.791574
H	4.816678	–0.007104	1.771536
H	2.244660	0.211895	2.300345
H	–3.253194	–1.918917	1.002752
H	–4.487738	–0.619880	0.891595
H	–3.169263	–0.529484	2.100010

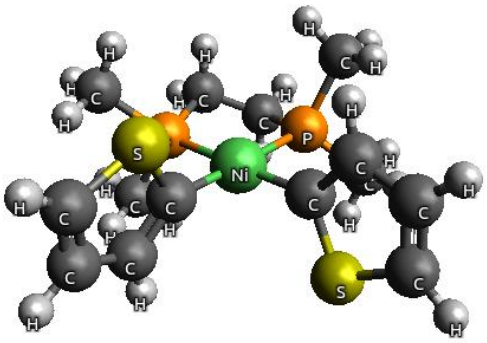




H	–2.738980	–1.555615	–1.914101
H	–4.093976	–0.384593	–1.804800
H	–2.538377	0.086096	–2.553890
H	–0.472015	2.498612	2.347530
H	0.286639	3.904367	1.543164
H	1.271147	2.482965	2.003736
H	1.027304	3.942623	–1.105713
H	2.208210	2.630960	–0.784212
H	1.073528	2.476905	–2.133820

$NiTh_2dmpe$

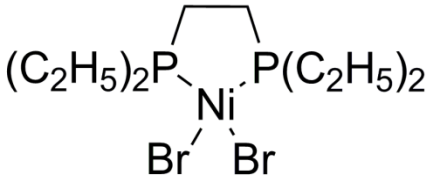


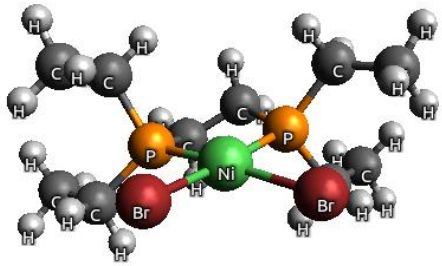


Ni	0.121724	0.022047	–0.001971
P	1.555571	1.742323	–0.182125
P	1.921873	–1.315457	0.142209
C	3.451835	–0.315213	–0.276715
C	3.280856	1.131891	0.222544
C	2.060013	–2.823802	–0.902527
C	2.247058	–1.952786	1.843055
C	1.352779	3.251557	0.850143
C	1.701232	2.421397	–1.891779
H	4.052540	1.793586	–0.187173
H	3.374926	1.167398	1.314680
H	4.361109	–0.776153	0.125630
H	3.542216	–0.328709	–1.369670
C	–3.236408	2.821770	0.562001
C	–3.013010	2.778717	–0.784435
C	–1.952367	1.881829	–1.147921
C	–1.362509	1.227180	–0.087940
S	–2.149755	1.737937	1.391734
H	–3.971865	3.398169	1.106798
H	–3.584394	3.358103	–1.503286
H	–1.658927	1.713141	–2.180326
C	–1.045463	–1.488707	0.128337
C	–1.461808	–2.229663	1.213338
C	–2.308651	–3.343299	0.890591
C	–2.540709	–3.465458	–0.449448
S	–1.727736	–2.192975	–1.323825
H	–1.196345	–1.976043	2.235871
H	–2.728455	–4.015272	1.632941
H	–3.141688	–4.200860	–0.967068
H	1.216932	–3.479020	–0.671465
H	3.001388	–3.353615	–0.727318
H	1.987537	–2.548000	–1.957716
H	1.384452	–2.548441	2.152062
H	3.149956	–2.570355	1.878489
H	2.352789	–1.118232	2.541454
H	1.995663	1.629742	–2.585994
H	0.717374	2.789985	–2.192710

H	2.429209	3.237042	–1.943511
H	0.388913	3.705363	0.609018
H	2.157194	3.972097	0.673154
H	1.335593	2.973938	1.906978

$NiBr_2depe$

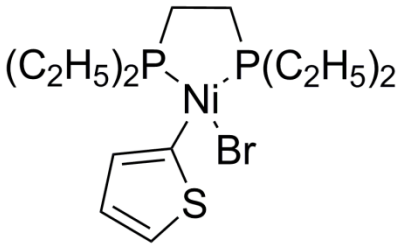


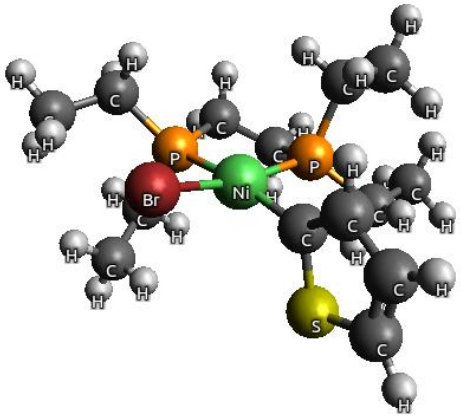


Ni	0.074816	–0.468839	0.078031
Br	–1.619264	–2.071947	–0.473627
Br	1.755713	–2.125070	0.504195
P	–1.439952	1.129277	–0.107094
C	–2.464163	1.372700	1.420409
C	–2.609633	1.134892	–1.534482
P	1.604072	1.097096	0.406619
C	2.669182	1.451563	–1.070657
C	2.734244	0.972562	1.859114
C	–0.539545	2.753735	–0.240856
C	0.716617	2.718519	0.647254
H	–1.192645	3.593853	0.028287
H	–0.258216	2.885594	–1.294643
H	1.378006	3.568105	0.433947
H	0.435347	2.784647	1.707203
H	3.175795	2.409236	–0.881650
C	3.691115	0.366455	–1.443163
H	1.979871	1.617860	–1.909902
C	–3.549481	2.347539	–1.634783
H	–1.984745	1.049587	–2.433915
H	–3.170746	0.196558	–1.473820
C	3.687116	2.158498	2.081690
H	3.283885	0.033174	1.738302
H	2.083226	0.825159	2.731616
H	–2.958806	2.350651	1.328435
H	–1.753202	1.454517	2.253906
C	–3.494507	0.273429	1.722358
H	4.245786	0.676858	–2.337455
H	3.202921	–0.591299	–1.644837
H	4.416052	0.201688	–0.637332
H	3.149412	3.102272	2.235272
H	4.295331	1.977761	2.976333
H	4.376021	2.291274	1.238977
H	–4.243645	0.193143	0.925925
H	–3.017106	–0.705625	1.822754
H	–4.019602	0.509088	2.656384
H	–3.001578	3.292564	–1.734832
H	–4.189072	2.243954	–2.519811
H	–4.208893	2.425918	–0.762223

NiBrThdepe

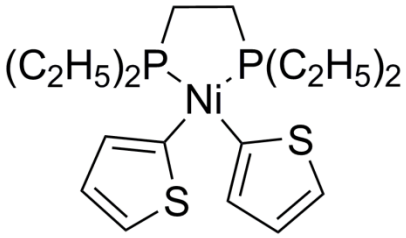
Ni	0.079800	0.275554	0.106070
P	–1.023952	–1.614712	0.078138
P	1.976677	–0.921652	–0.261529
Br	1.318241	2.262966	0.632354
C	1.520514	–2.729133	–0.164772
C	0.072940	–2.935131	–0.649492
C	3.490234	–0.856862	0.812136
C	2.576196	–0.787854	–2.016467
C	–2.629964	–1.783932	–0.815312
C	–1.321974	–2.283324	1.783355
H	–0.291205	–3.938942	–0.394058
H	0.016850	–2.837490	–1.742560
H	2.225141	–3.342560	–0.743213
H	1.616829	–3.036281	0.885505
C	–3.509379	2.592994	–0.915560
C	–3.508212	2.560318	0.457967
C	–2.416317	1.795420	0.997987
C	–1.573912	1.248415	0.049355
S	–2.160610	1.693777	–1.539536
H	–4.193067	3.109021	–1.581767
H	–4.248255	3.074219	1.068048
H	–2.239659	1.700193	2.067152
C	4.506966	0.255497	0.506905
H	3.976774	–1.841602	0.742217
H	3.120083	–0.746519	1.840177
C	2.668433	0.636776	–2.587674
H	3.545990	–1.303626	–2.082741
H	1.867298	–1.375324	–2.616963
H	–0.334805	–2.376578	2.255373
H	–1.716583	–3.303406	1.671941
C	–2.242388	–1.440899	2.678711
C	–3.284726	–3.174925	–0.801397
H	–3.300169	–1.027844	–0.390361
H	–2.437034	–1.455024	–1.844574
H	5.329886	0.206771	1.230991
H	4.941062	0.141359	–0.493831
H	4.039843	1.242131	0.578120
H	3.379401	1.255852	–2.032450
H	2.991285	0.595632	–3.635773
H	1.699428	1.144591	–2.541437
H	–2.638231	–3.942423	–1.244736
H	–3.547006	–3.495273	0.214031
H	–4.212921	–3.150342	–1.385421
H	–2.384667	–1.944403	3.642935
H	–3.229468	–1.291249	2.226396
H	–1.811513	–0.453534	2.867536

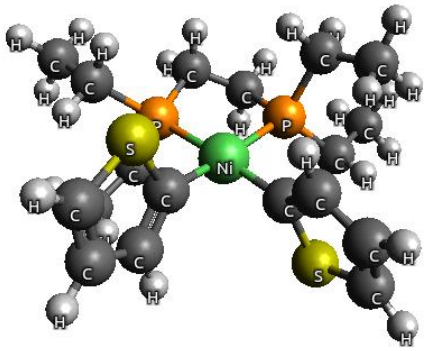




NiTh$_2$depe

Ni	–0.045055	0.153653	0.118213
P	1.684154	–1.311796	–0.205215
P	–1.411345	–1.669815	0.002499
C	–0.425208	–3.097614	–0.696162
C	1.008738	–3.059378	–0.141233
C	–2.993515	–1.686390	–0.965231
C	–1.875992	–2.300956	1.694936
C	3.170522	–1.379615	0.904859
C	2.373347	–1.220180	–1.935576
H	1.658861	–3.758268	–0.678896
H	1.013094	–3.364075	0.912239
H	–0.903197	–4.061323	–0.487520
H	–0.412939	–2.972535	–1.785726
C	2.651526	3.403918	1.391059
C	2.291661	3.703740	0.108332
C	1.411105	2.731839	–0.472926
C	1.096956	1.672110	0.348165
S	1.908540	1.905429	1.889017
H	3.284179	3.963933	2.066275
H	2.628767	4.595516	–0.411241
H	0.990295	2.841498	–1.467539
C	–1.500010	1.388620	0.210924
C	–2.084457	2.068436	1.255273
C	–3.153805	2.947304	0.876692
C	–3.390703	2.957448	–0.467924
S	–2.293974	1.869050	–1.280474
H	–1.734565	1.977964	2.279058
H	–3.711083	3.554321	1.583694
H	–4.118885	3.532445	–1.023708
C	–2.956147	–1.472198	2.403510
C	–3.781475	–3.001677	–0.986812
H	–0.953202	–2.291515	2.285905
H	–2.187517	–3.349131	1.607868
H	–2.727672	–1.375030	–1.981694
H	–3.600072	–0.868185	–0.565537
H	–4.693848	–2.882719	–1.580388
H	–3.205779	–3.818627	–1.432914
H	–4.084190	–3.314095	0.017381
H	–3.919520	–1.546434	1.889851
H	–3.098985	–1.835338	3.426415
H	–2.686595	–0.414425	2.444862
C	4.220575	–2.454295	0.596525
C	3.309527	–0.030987	–2.189368
H	3.610394	–0.378280	0.886611
H	2.777308	–1.503298	1.920786
H	5.044305	–2.391474	1.315220
H	4.649327	–2.331547	–0.402715
H	3.806178	–3.465372	0.661572
H	4.228564	–0.110526	–1.600376

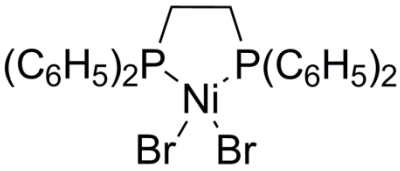


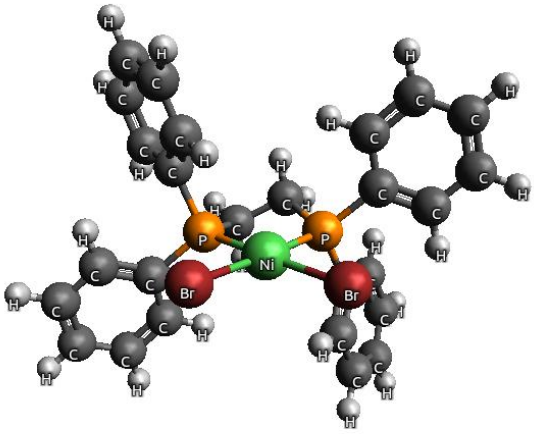


H	2.831070	0.916582	–1.931497
H	3.597172	–0.000342	–3.245396
H	2.880368	–2.166673	–2.159872
H	1.505565	–1.158823	–2.602291

$NiBr_2dppe$

Ni	0.004106	–0.001106	0.924463
Br	1.768800	–0.141923	2.531477
Br	–1.754769	0.151185	2.536519
P	1.538365	–0.105203	–0.659674
P	–1.534899	0.091741	–0.655432
C	0.695965	0.307606	–2.271841
C	–0.697700	–0.332978	–2.267178
H	1.294049	–0.030586	–3.125759
H	0.612583	1.398665	–2.337423
H	–1.298568	–0.001258	–3.121683
H	–0.614445	–1.424483	–2.324853
C	–2.162106	1.789383	–0.949381
C	–1.830462	2.823942	–0.056618
H	–1.258678	2.599847	0.841918
C	–2.262764	4.134731	–0.302404
H	–2.002947	4.924956	0.400446
C	–3.031509	4.423269	–1.437541
H	–3.368958	5.441866	–1.625838
C	–3.373397	3.393843	–2.329123
H	–3.978560	3.608971	–3.208822
C	–2.941421	2.085329	–2.086221
H	–3.227138	1.294459	–2.779795
C	2.991051	1.003347	–0.618711
C	4.275805	0.521605	–0.313248
H	4.429520	–0.536354	–0.113216
C	5.362319	1.401918	–0.244208
H	6.351198	1.015360	–0.001807
C	5.177094	2.772738	–0.469416
H	6.022688	3.456785	–0.409939
C	3.894823	3.262106	–0.757677
H	3.737679	4.327805	–0.918241
C	2.807538	2.383818	–0.827309
H	1.815591	2.789511	–1.024698
H	3.369444	–5.462285	–1.597024
C	3.032531	–4.442361	–1.415054
C	3.372679	–3.419170	–2.314431
H	3.975980	–3.640471	–3.193879
C	2.941396	–2.108944	–2.079664
H	3.225782	–1.322939	–2.779283
C	2.164575	–1.804997	–0.943233
C	1.834616	–2.833351	–0.042685
H	1.264777	–2.602992	0.855489

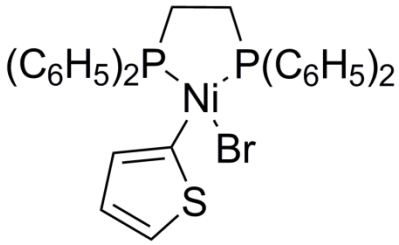


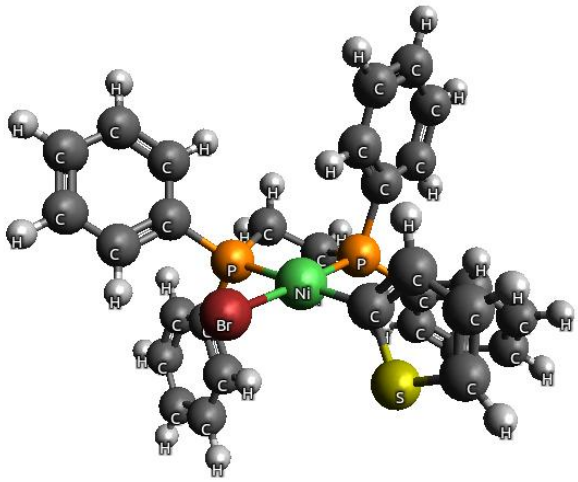


C	2.266179	–4.145880	–0.280343
H	2.007687	–4.931195	0.428472
H	–6.018318	–3.468386	–0.365673
C	–5.172942	–2.784775	–0.432769
C	–3.891437	–3.276289	–0.720826
H	–3.734680	–4.343188	–0.873605
C	–2.804406	–2.398528	–0.800244
H	–1.812978	–2.805701	–0.997268
C	–2.987438	–1.016497	–0.601750
C	–4.271376	–0.532470	–0.296497
H	–4.424623	0.527009	–0.104298
C	–5.357638	–1.412276	–0.217633
H	–6.345869	–1.023905	0.024520

NiBrThdppe

Ni	0.034482	–0.134585	0.789592
P	1.304752	0.283769	–0.944308
P	–1.752129	–0.053268	–0.621326
Br	–1.381129	–0.481373	2.684557
C	–1.118265	0.597502	–2.249729
C	0.283134	0.011194	–2.481770
H	0.769781	0.457957	–3.357394
H	0.204256	–1.069460	–2.649601
H	–1.796384	0.350143	–3.074825
H	–1.051941	1.689583	–2.184003
C	3.551104	–1.160228	3.232338
C	3.463800	0.210944	3.278962
C	2.372282	0.723144	2.495415
C	1.616797	–0.250965	1.866181
S	2.283672	–1.815464	2.245626
H	4.259042	–1.811113	3.735307
H	4.141256	0.835415	3.857732
H	2.142744	1.784828	2.432410
H	–6.164514	0.614323	1.522718
C	–5.410260	1.067482	0.881017
C	–4.264635	0.338090	0.545015
H	–4.135421	–0.668525	0.935981
C	–3.273042	0.906146	–0.279282
C	–3.444593	2.225274	–0.739270
H	–2.690259	2.702100	–1.362342
C	–4.592962	2.953826	–0.401910
H	–4.711483	3.971891	–0.770735
C	–5.580130	2.376826	0.408109
H	–6.471722	2.943991	0.672880
H	–3.497911	–5.346706	–1.998170
C	–3.174662	–4.340043	–1.735143
C	–2.217798	–4.148598	–0.730240
H	–1.795698	–5.003092	–0.203216

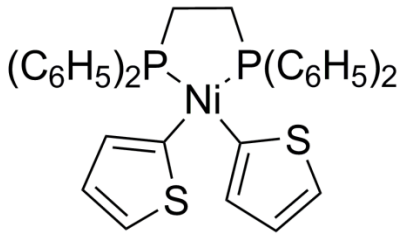




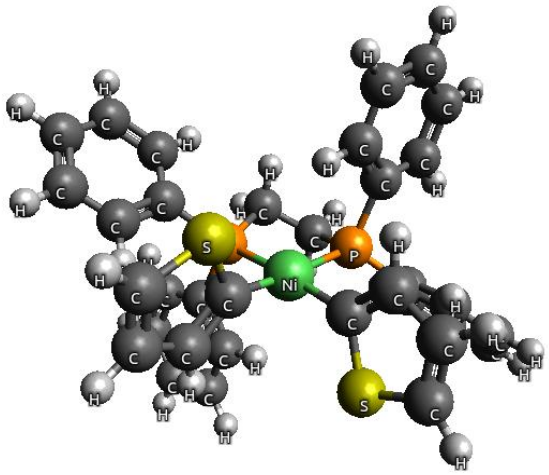
C	–1.804439	–2.852883	–0.388475
H	–1.082135	–2.707253	0.412831
C	–2.344542	–1.737428	–1.052386
C	–3.314572	–1.937122	–2.054962
H	–3.764583	–1.082582	–2.560754
C	–3.725976	–3.229978	–2.396129
H	–4.478996	–3.372104	–3.170336
H	4.245484	–3.116930	–3.119528
C	4.194449	–2.297337	–2.404042
C	5.336228	–1.909317	–1.691252
H	6.282199	–2.425887	–1.849449
C	5.251912	–0.857537	–0.766935
H	6.128616	–0.558311	–0.194601
C	4.037448	–0.197349	–0.557336
H	3.979993	0.597999	0.182609
C	2.887595	–0.572055	–1.279978
C	2.977053	–1.634701	–2.198052
H	2.106001	–1.962805	–2.761200
C	1.696903	2.075328	–1.034825
C	1.098322	2.959221	–0.119044
H	0.459033	2.567814	0.672169
C	1.326903	4.338779	–0.211584
H	0.859996	5.011138	0.506868
C	2.159709	4.847031	–1.217505
H	2.342078	5.918835	–1.286861
C	2.765590	3.970434	–2.131582
H	3.419395	4.359193	–2.911284
C	2.535481	2.592826	–2.040879
H	3.021295	1.920239	–2.747530

$NiTh_2dppe$

Ni	–0.004384	–0.004569	0.726972
P	1.541817	0.255990	–0.913976
P	–1.535345	–0.229696	–0.931628
C	–0.717438	0.284566	–2.526412
C	0.735635	–0.218288	–2.527410
H	1.287560	0.184103	–3.385842
H	0.747516	–1.313757	–2.594860
H	–1.263415	–0.094740	–3.399045
H	–0.727678	1.381419	–2.565921
C	3.002225	–0.749421	3.858117
C	2.929640	0.618751	3.744637
C	1.970654	1.045561	2.761062
C	1.307062	0.013406	2.119811
S	1.880460	–1.502806	2.767002
H	3.622150	–1.343404	4.521824
H	3.528122	1.301414	4.344553
H	1.772051	2.095121	2.551941



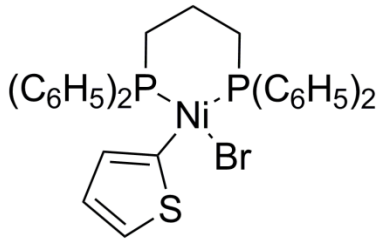
C	–1.333375	–0.049926	2.102749
C	–1.999971	–1.094024	2.721175
C	–2.969018	–0.685549	3.702701
C	–3.047525	0.680407	3.836376
S	–1.918944	1.454247	2.766912
H	–1.795207	–2.139644	2.498741
H	–3.570257	–1.379375	4.286851
H	–3.675696	1.262115	4.503199
C	3.187227	–0.550548	–0.967134
C	4.069776	–0.353992	0.114620
H	3.766012	0.256309	0.963127
C	5.334982	–0.951196	0.112128
H	6.000886	–0.791273	0.958848
C	5.736552	–1.761048	–0.960464
H	6.720513	–2.228714	–0.956335
C	4.861914	–1.969861	–2.034901
H	5.160839	–2.598734	–2.872690
C	3.596215	–1.367858	–2.038466
H	2.940717	–1.545676	–2.887942
C	–1.885052	–2.013997	–1.208354
C	–2.877319	–2.446971	–2.108427
H	–3.500920	–1.717995	–2.625644
C	–3.083501	–3.813256	–2.332705
H	–3.857486	–4.136196	–3.027987
C	–2.300404	–4.763747	–1.658685
H	–2.464009	–5.826935	–1.831247
C	–1.315169	–4.340945	–0.756310
H	–0.709577	–5.071580	–0.221719
C	–1.111359	–2.973188	–0.529837
H	–0.353738	–2.649936	0.183708
H	0.705291	5.081618	–0.112113
C	1.319636	4.362549	–0.652375
C	2.320220	4.804522	–1.528352
H	2.486942	5.871159	–1.674658
C	3.114699	3.868666	–2.209425
H	3.900635	4.206413	–2.883959
C	2.904473	2.497842	–2.018850
H	3.536688	1.779893	–2.540965
C	1.896837	2.045832	–1.145692
C	1.111954	2.990280	–0.459316
H	0.342683	2.651820	0.234447
H	–6.023427	0.738461	0.913807
C	–5.345923	0.930707	0.083179
C	–5.733899	1.779326	–0.964225
H	–6.718894	2.244776	–0.956879
C	–4.844383	2.029745	–2.017258
H	–5.132724	2.688900	–2.835241
C	–3.577280	1.430636	–2.024994
H	–2.910184	1.641197	–2.857787
C	–3.182059	0.574394	–0.979276
C	–4.079620	0.336073	0.081479

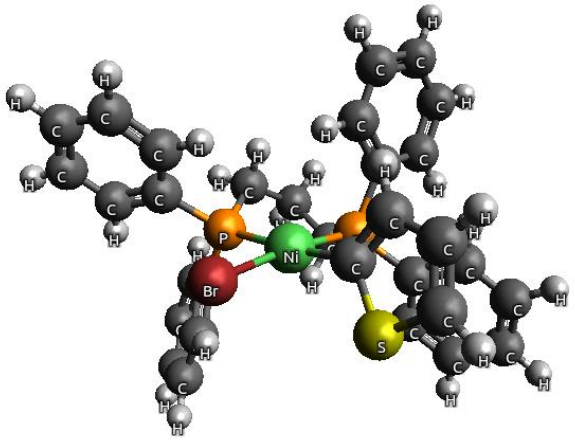


H	–3.786236	–0.304300	0.911280

NiBrThdppp

Ni	–0.018096	–0.007691	0.755791
P	1.304421	0.398854	–0.915187
P	–1.843377	0.205349	–0.527767
Br	–1.335190	–0.527233	2.634659
C	–1.650647	1.387797	–1.935481
C	0.554219	0.114873	–2.579920
H	1.353181	0.157318	–3.332829
H	0.185900	–0.921721	–2.569892
H	–2.625599	1.543642	–2.416402
H	–1.409117	2.340477	–1.441222
C	3.526768	–1.227121	3.009588
C	3.528182	0.141093	3.066324
C	2.427048	0.723687	2.359845
C	1.579694	–0.197345	1.781774
S	2.162190	–1.796458	2.110128
H	4.223603	–1.925310	3.461036
H	4.280385	0.716367	3.601129
H	2.263444	1.799620	2.303597
H	–6.617425	0.049131	0.905085
C	–5.701116	0.635501	0.868990
C	–4.564323	0.101770	0.258126
H	–4.599641	–0.900824	–0.168112
C	–3.378700	0.840258	0.218097
C	–3.336520	2.110890	0.809498
H	–2.400444	2.673609	0.833364
C	–4.472913	2.645567	1.410805
H	–4.427916	3.629175	1.874472
C	–5.660123	1.907747	1.440069
H	–6.545998	2.319619	1.920172
H	–2.970298	–4.840932	–2.951382
C	–2.775348	–3.874987	–2.488674
C	–1.966660	–3.794219	–1.352981
H	–1.534198	–4.695239	–0.922514
C	–1.711769	–2.554810	–0.763764
H	–1.085004	–2.487824	0.129762
C	–2.268388	–1.387192	–1.305306
C	–3.089440	–1.477294	–2.438799
H	–3.543070	–0.577801	–2.859868
C	–3.338611	–2.715286	–3.030789
H	–3.974543	–2.776534	–3.912067
H	3.833916	–3.685365	–2.019245
C	3.903312	–2.676119	–1.618005
C	5.120451	–2.193274	–1.132520
H	6.006870	–2.824643	–1.156161
C	5.193892	–0.902596	–0.605134

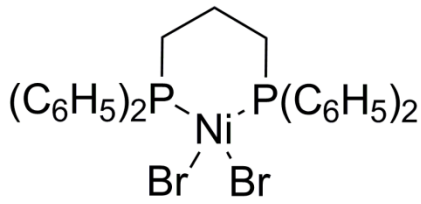


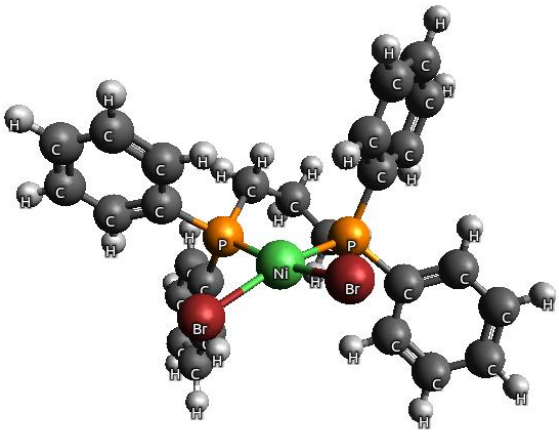


H	6.135086	–0.525362	–0.210019
C	4.058573	–0.093836	–0.563963
H	4.122200	0.900852	–0.123202
C	2.838227	–0.569662	–1.056213
C	2.767452	–1.869892	–1.576559
H	1.818290	–2.275121	–1.931659
C	1.777749	2.155538	–0.970469
C	1.226550	3.030186	–0.025804
H	0.575322	2.629008	0.756712
C	1.507378	4.395773	–0.080726
H	1.078627	5.067496	0.660471
C	2.343945	4.895034	–1.080929
H	2.567660	5.959508	–1.123189
C	2.899064	4.027192	–2.026739
H	3.554765	4.414576	–2.804320
C	2.616494	2.662759	–1.972724
H	3.059164	1.989187	–2.708971
C	–0.580764	1.058251	–2.990022
H	–1.069045	0.606145	–3.863604
H	–0.144927	2.004632	–3.338799

$NiBr_2dppp$

Ni	–0.028290	0.104407	0.824957
P	1.576684	0.019499	–0.671505
P	–1.580450	–0.193187	–0.698970
Br	–1.692761	–0.219375	2.464777
C	–1.093797	0.458879	–2.355676
C	1.096445	–0.930428	–2.180148
H	1.998457	–1.163922	–2.761290
H	0.726957	–1.892892	–1.794327
H	–1.985714	0.510125	–2.994208
H	–0.806397	1.503152	–2.161714
H	–6.497843	0.368861	–0.144135
C	–5.528940	0.862736	–0.187515
C	–4.376083	0.103602	–0.396002
H	–4.450897	–0.979026	–0.500035
C	–3.126724	0.728525	–0.436599
C	–3.036617	2.114982	–0.253808
H	–2.058968	2.602772	–0.230921
C	–4.189109	2.870759	–0.052018
H	–4.111031	3.945705	0.098566
C	–5.439211	2.245078	–0.020761
H	–6.338630	2.834093	0.148915
H	–2.887052	–5.668955	–1.645800
C	–2.648464	–4.622377	–1.464873
C	–1.979877	–4.248308	–0.297543
H	–1.701578	–4.999374	0.439032
C	–1.672618	–2.906862	–0.065295

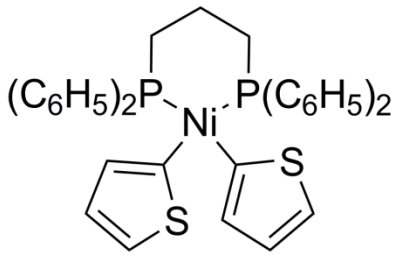




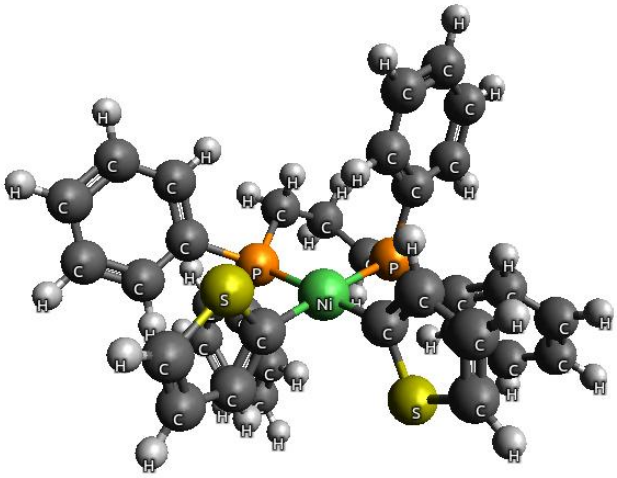
H	–1.172711	–2.603642	0.857492
C	–2.032318	–1.929745	–1.003292
C	–2.712213	–2.310498	–2.169963
H	–3.017456	–1.558470	–2.899895
C	–3.017200	–3.651275	–2.400902
H	–3.546780	–3.938074	–3.307437
H	3.729705	–4.015423	1.108819
C	3.903784	–3.006940	0.738791
C	5.199309	–2.483047	0.707610
H	6.039874	–3.086433	1.045303
C	5.410215	–1.177951	0.260579
H	6.414534	–0.758527	0.253887
C	4.334286	–0.396962	–0.165649
H	4.503804	0.631338	–0.485911
C	3.040110	–0.923514	–0.147004
C	2.828456	–2.228775	0.317866
H	1.814552	–2.629562	0.387443
C	2.142658	1.621951	–1.318952
C	1.746227	2.800574	–0.673924
H	1.151689	2.735587	0.239965
C	2.138833	4.041305	–1.178201
H	1.832250	4.951732	–0.667130
C	2.930075	4.112097	–2.326239
H	3.238959	5.079967	–2.717241
C	3.331344	2.939111	–2.973294
H	3.951685	2.990829	–3.866082
C	2.938703	1.698572	–2.472291
H	3.260575	0.787881	–2.981721
C	0.038638	–0.283238	–3.076220
H	–0.392141	–1.074224	–3.704615
H	0.525106	0.424610	–3.760426
Br	1.602019	0.797202	2.384156

$NiTh_2dppp$

Ni	0.000294	–0.174748	0.532034
P	1.590378	0.415309	–0.900721
P	–1.581281	0.217423	–0.974527
C	–1.143119	1.457090	–2.270916
C	1.144535	0.198971	–2.679507
H	2.037051	0.329985	–3.306399
H	0.847876	–0.856641	–2.768564
H	–2.035683	1.702823	–2.862086
H	–0.877817	2.365603	–1.710424
C	2.966050	–2.014882	3.162694
C	2.811042	–0.741331	3.640527
C	1.853949	0.020770	2.894711
C	1.285372	–0.661446	1.841862
S	1.938488	–2.269815	1.789027

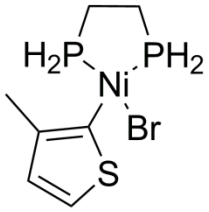


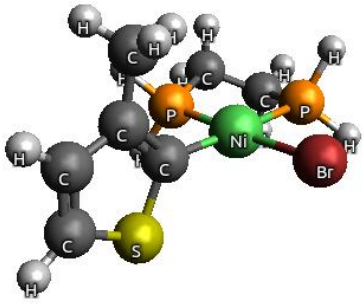
H	3.602070	–2.809987	3.536786
H	3.348027	–0.360942	4.506525
H	1.568167	1.040261	3.154348
H	–6.094663	–0.405044	0.939956
C	–5.366332	0.321718	0.585583
C	–4.167214	–0.121142	0.030700
H	–3.966987	–1.190519	–0.037747
C	–3.211681	0.800960	–0.415643
C	–3.470714	2.172285	–0.285458
H	–2.729482	2.909544	–0.597120
C	–4.673031	2.614160	0.266275
H	–4.861835	3.681798	0.362732
C	–5.622759	1.689714	0.705385
H	–6.557673	2.034542	1.143556
H	–2.553645	–4.611029	–3.870247
C	–2.375569	–3.687701	–3.321657
C	–1.433629	–3.657939	–2.291528
H	–0.875988	–4.555379	–2.030661
C	–1.210736	–2.474476	–1.585900
H	–0.480087	–2.448117	–0.771431
C	–1.926646	–1.313465	–1.906044
C	–2.874021	–1.352185	–2.938629
H	–3.452041	–0.458194	–3.181234
C	–3.096987	–2.533669	–3.644635
H	–3.836521	–2.558124	–4.442929
H	4.918492	–3.101798	–1.966557
C	4.707350	–2.213324	–1.374248
C	5.633764	–1.760809	–0.432892
H	6.571535	–2.294682	–0.289311
C	5.350314	–0.625153	0.330454
H	6.060183	–0.275407	1.077503
C	4.147313	0.055168	0.154259
H	3.917673	0.923334	0.773212
C	3.218154	–0.388173	–0.796417
C	3.502777	–1.532887	–1.552190
H	2.782949	–1.913743	–2.277776
C	1.939478	2.198417	–0.739237
C	1.228917	2.939825	0.214016
H	0.511922	2.430036	0.865351
C	1.440618	4.313938	0.339029
H	0.888531	4.880201	1.086678
C	2.364038	4.954500	–0.489383
H	2.530605	6.026008	–0.392991
C	3.081455	4.219479	–1.439371
H	3.806900	4.716847	–2.080611
C	2.871689	2.846619	–1.561590
H	3.444024	2.273411	–2.293947
C	0.013466	1.088918	–3.215666
H	–0.401250	0.585705	–4.099617
H	0.448875	2.030160	–3.577783
C	–1.292176	–0.585916	1.860921



C	–1.863823	–1.766076	2.282966
C	–2.819056	–1.610920	3.339842
C	–2.970778	–0.308614	3.733656
S	–1.938649	0.724529	2.798553
H	–1.583595	–2.734174	1.867417
H	–3.359289	–2.437140	3.796392
H	–3.607543	0.098617	4.511710

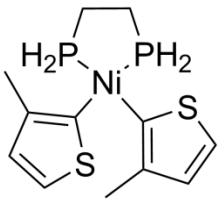
NiBrMeThdhpe





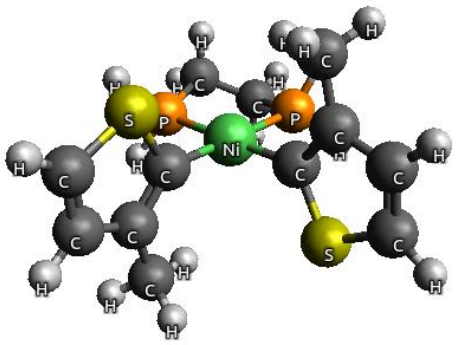
Ni	0.445733	–0.244810	–0.150688
P	0.860958	1.786998	0.395004
P	2.656919	–0.611805	–0.191005
Br	–0.011081	–2.514505	–0.685913
C	3.517084	1.047823	–0.108585
C	2.683076	2.011233	0.766565
H	3.293213	–1.260859	–1.267470
H	3.237044	–1.331667	0.877483
H	0.223780	2.367707	1.507812
H	0.583885	2.769865	–0.578454
H	2.999034	3.051897	0.626701
H	2.816480	1.767178	1.829093
H	4.544414	0.965713	0.264342
H	3.570109	1.424078	–1.138872
C	–3.682867	1.116056	–0.803430
C	–3.604840	0.782349	0.525898
C	–2.295540	0.337418	0.931417
C	–1.387980	0.321515	–0.114610
S	–2.154081	0.874772	–1.583929
H	–4.544574	1.465151	–1.363082
H	–4.454080	0.841089	1.204656
C	–1.986117	–0.117565	2.338328
H	–2.447738	–1.092992	2.544981
H	–0.906354	–0.240306	2.485211
H	–2.363567	0.592229	3.087632

NiMeTh$_2$dhpe

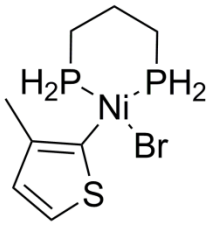


Ni	0.620075	0.004161	–0.000620
P	2.229480	1.540393	0.059654
P	2.241978	–1.518270	–0.060677
C	3.888952	–0.674023	–0.345045
C	3.882735	0.709124	0.346512
H	2.250129	–2.568232	–1.002337
H	2.474146	–2.279903	1.108125
H	2.228896	2.591090	1.000566
H	2.457400	2.303101	–1.109344

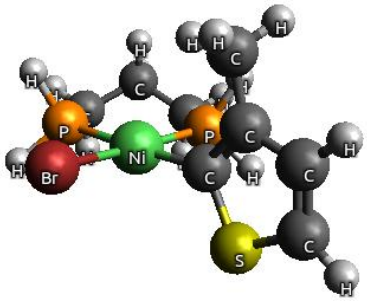
H	4.722043	1.326038	0.005421
H	3.985116	0.586649	1.433220
H	4.732635	–1.284058	–0.002363
H	3.992362	–0.550744	–1.431562
C	–2.412629	3.074800	0.883328
C	–2.271597	3.066255	–0.481208
C	–1.319027	2.093253	–0.957971
C	–0.738117	1.356744	0.061172
S	–1.380858	1.877161	1.601467
H	–3.057846	3.697695	1.494315
H	–2.830796	3.728333	–1.140703
C	–1.034805	1.892183	–2.429221
C	–0.723728	–1.362822	–0.060947
C	–1.292791	–2.107800	0.958791
C	–2.235931	–3.090570	0.483376
C	–2.381264	–3.098291	–0.880729
S	–1.366552	–1.886840	–1.599918
C	–1.006226	–1.905805	2.429458
H	–2.785159	–3.760364	1.143449
H	–3.021061	–3.727651	–1.490791
H	–0.158061	–1.226193	2.574578
H	–1.868344	–1.460322	2.945543
H	–0.776398	–2.855651	2.932975
H	–0.185381	1.214540	–2.575931
H	–0.807991	2.842629	–2.933054
H	–1.896899	1.445003	–2.943859



NiBrMeThdhpp



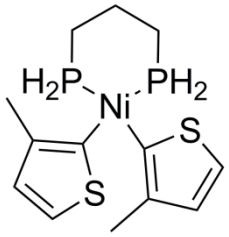
Ni	0.305098	–0.156255	–0.006371
P	0.762343	1.923841	0.297590
P	2.423221	–0.886180	–0.123392
Br	–0.362459	–2.393341	–0.504943
C	2.506422	2.465544	0.656700
H	2.789823	–1.322794	–1.413834
H	2.753355	–2.043284	0.608384
H	0.041611	2.605456	1.296173
H	0.438034	2.720766	–0.820269
H	2.574998	3.544467	0.466707
H	2.677955	2.318476	1.732217
C	–3.815962	1.156145	0.793337
C	–3.616183	1.347873	–0.550569
C	–2.291183	0.988927	–0.991998
C	–1.494559	0.511794	0.035758
S	–2.385488	0.518492	1.538467
H	–4.716639	1.328377	1.373705
H	–4.388172	1.724882	–1.219387
C	3.592324	1.717153	–0.147608
C	3.827102	0.257928	0.304271

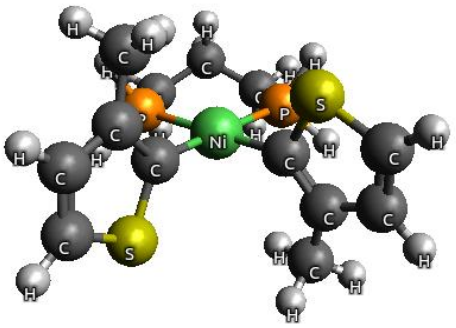


H	3.954131	0.229402	1.395461
H	4.755158	–0.126726	–0.136062
H	3.358359	1.749216	–1.223108
H	4.536689	2.264420	–0.030201
C	–1.863033	1.079945	–2.438049
H	–2.436829	0.378962	–3.059533
H	–2.021204	2.087766	–2.848145
H	–0.805554	0.816684	–2.553073

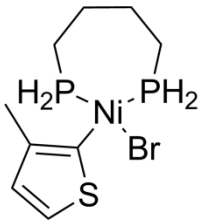
NiMeTh$_2$dhpp

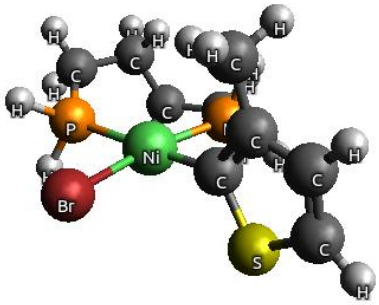
Ni	0.568578	–0.025842	0.003972
P	2.029567	1.608345	–0.300669
P	2.061917	–1.611398	0.392132
C	3.876066	–1.300094	0.104273
C	4.338128	0.120302	0.505713
H	1.880591	–2.856329	–0.245631
H	2.058559	–2.060362	1.731729
H	2.010743	2.575259	0.729675
H	1.824794	2.466558	–1.400716
H	5.436048	0.130217	0.504878
H	4.037547	0.337784	1.542491
H	4.463036	–2.052002	0.646148
H	4.066383	–1.455432	–0.967051
C	–2.491439	2.810359	–1.416997
C	–2.340373	3.068882	–0.078278
C	–1.376616	2.212718	0.569481
C	–0.797004	1.293777	–0.291307
S	–1.457557	1.501209	–1.897542
H	–3.145625	3.299497	–2.131496
H	–2.898798	3.843858	0.444616
C	–0.781102	–1.354466	0.333083
C	–1.323787	–2.305043	–0.518196
C	–2.300532	–3.150288	0.121775
C	–2.499466	–2.851793	1.446560
S	–1.495529	–1.518586	1.920372
H	–2.832906	–3.947374	–0.394977
H	–3.168476	–3.329460	2.155030
C	3.852526	1.245757	–0.437176
H	4.050286	0.958660	–1.479507
H	4.419548	2.165288	–0.246027
C	–1.084575	2.300218	2.050262
C	–0.979217	–2.429719	–1.984830
H	–0.222956	1.677579	2.318750
H	–0.875682	3.332929	2.364090
H	–1.937486	1.942522	2.644091
H	–0.829066	–3.477700	–2.280208
H	–0.066452	–1.869814	–2.223889
H	–1.779989	–2.020756	–2.617134





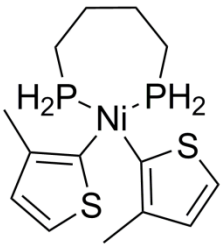
NiBrMeThdhpb





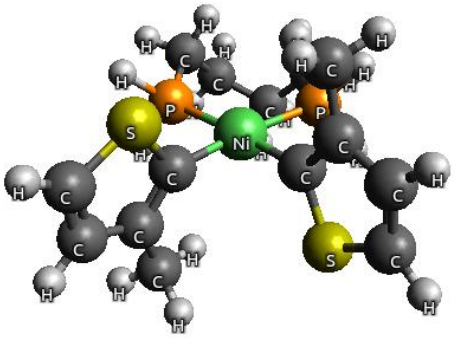
P	–0.648008	–1.899973	0.216545
P	–2.185520	1.251944	–0.107893
Br	0.751148	2.434697	–0.075459
C	–3.800644	–1.069908	–0.506542
H	–2.181240	2.373862	–0.954871
H	–2.507113	1.910465	1.098643
H	0.274709	–2.660424	0.954900
H	–0.532988	–2.565246	–1.023475
H	–4.783992	–1.449258	–0.812835
H	–3.090803	–1.449322	–1.255784
C	3.925825	–1.366075	0.556236
C	3.660207	–1.427117	–0.788114
C	2.343194	–0.951761	–1.136231
C	1.622328	–0.522758	–0.034421
S	2.571042	–0.707682	1.417968
H	4.837344	–1.639724	1.077688
H	4.378398	–1.789511	–1.521822
C	–2.249792	–2.594551	0.901875
C	–3.820375	0.466059	–0.584453
C	–3.433480	–1.614264	0.897412
H	–2.494762	–3.502369	0.334364
H	–2.034152	–2.909139	1.931138
H	–4.045846	0.785272	–1.609810
H	–4.609759	0.875054	0.058991
H	–4.300055	–2.118314	1.344293
H	–3.196704	–0.780628	1.573968
Ni	–0.144848	0.220671	0.014588
C	1.852557	–0.890387	–2.564168
H	2.448086	–0.177595	–3.150977
H	0.810784	–0.552966	–2.609330
H	1.924768	–1.867428	–3.063383

NiMeTh$_2$dhpb



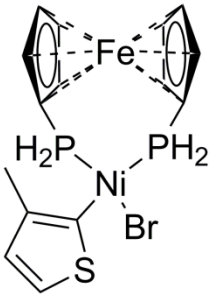
Ni	0.378368	0.081883	–0.085779
P	1.650027	1.883733	0.198112
P	1.926075	–1.456980	–0.524670
C	3.691172	–1.062717	–0.969780
C	4.048985	0.633614	1.018597
H	1.578445	–2.292061	–1.605762
H	2.087297	–2.453381	0.465222
H	1.394738	2.495026	1.443980
H	1.379121	2.990626	–0.635701
H	4.862899	0.968630	1.673812

H	3.266195	0.259840	1.696122
H	4.154751	–1.958007	–1.403832
H	3.628475	–0.323510	–1.780751
C	–2.897767	2.643277	1.395211
C	–2.807688	2.884608	0.047378
C	–1.780239	2.114154	–0.608098
C	–1.087083	1.279339	0.255686
S	–1.726400	1.456467	1.874004
H	–3.576946	3.084031	2.117831
H	–3.453605	3.588394	–0.475422
C	–0.874987	–1.368011	–0.233102
C	–1.283836	–2.301893	0.706618
C	–2.218600	–3.266432	0.180433
C	–2.517585	–3.073752	–1.144526
S	–1.661797	–1.694798	–1.760081
H	–2.649628	–4.069116	0.776954
H	–3.185962	–3.647571	–1.778347
C	3.514056	1.846456	0.212995
H	3.865760	1.813046	–0.826467
H	3.880488	2.788988	0.637015
C	4.589709	–0.538006	0.170115
H	4.823942	–1.369701	0.849742
H	5.545174	–0.234795	–0.281584
C	–0.850320	–2.305177	2.155025
C	–1.537605	2.191920	–2.098193
H	–0.599040	1.694870	–2.371714
H	–1.492430	3.232544	–2.449140
H	–2.340869	1.690909	–2.656734
H	–1.670054	–1.986113	2.814108
H	–0.535064	–3.305787	2.483254
H	–0.017610	–1.610917	2.319146

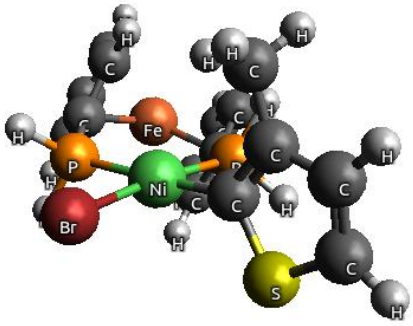


NiBrMeThdhpf

Ni	1.154420	0.403668	0.019627
Br	2.576095	2.318706	0.137326
P	–0.556158	1.900583	0.028987
P	0.091682	–1.494542	0.031475
C	4.637051	–2.261838	0.405434
C	4.394410	–2.132470	–0.938666
C	3.258154	–1.296291	–1.238827
C	2.651899	–0.789733	–0.101093
S	3.486069	–1.347864	1.326270
H	5.429548	–2.815611	0.898371
H	5.006427	–2.607773	–1.703429
C	–3.922121	–2.226590	0.445218
C	–2.700880	–2.316822	–0.291177
C	–1.665540	–1.672334	0.472607
C	–2.265229	–1.196862	1.692384

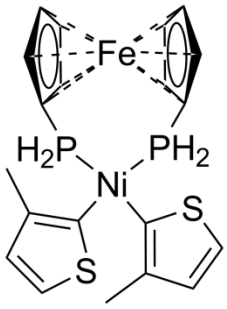


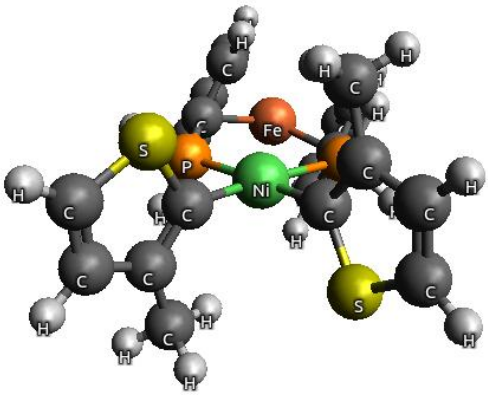
C	–3.652832	–1.538147	1.669880
H	–4.888850	–2.595080	0.119026
H	–2.576830	–2.773202	–1.268051
H	–1.753147	–0.661484	2.485812
H	–4.378432	–1.294251	2.438421
Fe	–3.149401	–0.320011	0.046343
C	–2.276133	1.485328	–0.399876
C	–3.462038	1.705016	0.383143
C	–4.577280	1.166801	–0.330354
C	–4.095655	0.622523	–1.562288
C	–2.680476	0.816754	–1.609727
H	–3.496768	2.176174	1.360166
H	–5.605621	1.153642	0.014675
H	–4.693961	0.125918	–2.318628
H	–2.021379	0.503138	–2.413383
H	–0.332924	3.048639	–0.755824
H	–0.749461	2.522957	1.279965
H	0.676933	–2.491581	0.834015
H	0.110157	–2.151489	–1.216014
C	2.834297	–0.977934	–2.653622
H	2.687071	–1.889297	–3.250672
H	3.596652	–0.371835	–3.162055
H	1.903978	–0.398421	–2.666395



NiMeTh$_2$dhpf

Ni	0.920765	–0.000510	–0.000405
P	–0.494013	1.730547	0.047301
P	–0.496826	–1.729435	–0.045999
C	4.007449	–3.100650	0.566536
C	3.824690	–2.986598	–0.788117
C	2.848835	–1.989899	–1.156197
C	2.291153	–1.343319	–0.063816
S	2.988345	–1.975771	1.408997
H	4.676445	–3.763026	1.106321
H	4.367801	–3.588779	–1.514854
C	4.015234	3.090092	–0.576294
C	3.835685	2.976718	0.778850
C	2.858116	1.982709	1.149626
C	2.295389	1.337948	0.058744
S	2.990355	1.968355	–1.415933
H	4.684776	3.750399	–1.117932
H	4.382561	3.577318	1.504074
C	–4.589467	–1.734815	0.297732
C	–3.394805	–2.028005	–0.430600
C	–2.268211	–1.635275	0.371350
C	–2.786709	–1.106209	1.606306
C	–4.213894	–1.170250	1.557384
H	–5.603223	–1.891797	–0.054859





H	–3.343724	–2.453499	–1.427689
H	–2.194864	–0.717594	2.429184
H	–4.891904	–0.825561	2.330681
Fe	–3.462850	0.003114	0.000967
C	–2.265542	1.639205	–0.369785
C	–3.391056	2.034038	0.432719
C	–4.586566	1.743125	–0.295090
C	–4.212606	1.178025	–1.554989
C	–2.785565	1.111351	–1.604610
H	–3.338665	2.459107	1.429921
H	–5.599883	1.901740	0.058026
H	–4.891604	0.834690	–2.328019
H	–2.194837	0.721841	–2.427862
H	–0.086778	2.849369	–0.708375
H	–0.567931	2.348238	1.315199
H	–0.091042	–2.847783	0.711126
H	–0.571540	–2.348432	–1.313152
C	2.535847	1.665484	2.592414
C	2.523221	–1.672034	–2.598087
H	2.348967	2.577344	3.177094
H	3.365347	1.129492	3.074868
H	1.650868	1.022352	2.667037
H	1.640970	–1.024884	–2.670089
H	3.353566	–1.140128	–3.083575
H	2.330263	–2.583357	–3.181655