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Supplementary Material

Table I: LDA/BP NLSCF optimized cartesian coordinates for the supine η^4-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**1a**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.12087	0.10202	0.00000
C	-2.04709	-0.54748	0.00000
C	-1.75004	0.13084	1.20910
C	-1.75004	0.13084	-1.20910
H	-2.18269	-1.63623	0.00000
H	-1.74678	-0.40430	2.16353
H	-1.74678	-0.40430	-2.16353
H	-1.88803	1.22141	1.27195
H	-1.88803	1.22141	-1.27195
C	1.63415	-0.66690	0.73274
C	1.63415	-0.66690	-0.73274
C	1.41996	0.48907	1.47620
C	1.41996	0.48907	-1.47620
H	1.25246	0.42141	2.55507
H	1.25246	0.42141	-2.55507
H	1.65407	1.49148	1.09445
H	1.65407	1.49148	-1.09445
H	1.59954	-1.64218	1.23302
H	1.59954	-1.64218	-1.23302

Table II: LDA/BP NLSCF optimized cartesian coordinates for the supine η^2-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**1b**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.25625	-0.23791	0.29277
C	-1.76810	-0.21513	1.52312
C	-2.23897	-0.62085	0.22429
C	-1.93433	0.24990	-0.83123
C	1.32563	0.05877	1.53899
C	1.49437	-1.18744	0.92598
C	1.26438	-2.52333	1.49698
C	1.19762	-2.80160	2.82093
H	-1.82621	0.84449	1.82051
H	-1.72675	-0.94603	2.34110
H	-2.52129	-1.66383	0.03035
H	0.99484	0.14934	2.58039
H	1.80154	0.94930	1.10470
H	1.97631	-1.19089	-0.07050
H	1.21713	-3.34762	0.77213
H	1.31520	-2.02861	3.59128
H	1.05604	-3.83082	3.17069
H	-1.99986	-0.09330	-1.87125
H	-1.86729	1.33757	-0.67420

Table III: LDA/BP NLSCF optimized cartesian coordinates for the supine transition state of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**1c**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.02669	-1.19523	-1.70027
C	-1.37171	-1.25625	0.06797

C	-1.87820	-1.40005	-1.35010
C	-1.91754	-0.37488	-2.28700
C	1.31694	0.36476	-2.07798
C	1.97631	-0.75028	-1.50533
C	1.41702	-1.40745	-0.35843
C	0.32805	-0.87685	0.50827
H	-2.19756	-2.40484	-1.66643
H	0.85376	1.14573	-1.46100
H	1.56174	0.66039	-3.10447
H	2.73990	-1.29275	-2.07621
H	1.80669	-2.40905	-0.12762
H	-1.82196	-0.38096	0.56000
H	-1.58011	-2.17061	0.63657
H	0.33819	0.21728	0.60199
H	0.34922	-1.34561	1.50316
H	-1.78855	0.67851	-2.00979
H	-2.30247	-0.57217	-3.29287

Table IV: LDA/BP NLSCF optimized cartesian coordinates for the supine product of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**1d**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.16205	-0.93449	-2.48940
C	-1.47707	-0.96325	-0.26815
C	-1.73493	-1.46296	-1.67537
C	-1.87725	-0.70035	-2.82212
C	1.74951	0.07047	-1.74336
C	1.87725	-1.32046	-1.54866
C	0.76809	-1.99140	-0.92060
C	-0.10595	-1.54455	0.25136
H	-1.87277	-2.55110	-1.77386
H	1.25817	0.72557	-1.01090
H	2.40156	0.57080	-2.47272
H	2.60975	-1.90150	-2.12083
H	0.71021	-3.06736	-1.15151
H	-1.45211	0.13902	-0.24793
H	-2.29706	-1.29486	0.39396
H	0.40016	-0.79787	0.88450
H	-0.29461	-2.43232	0.87931
H	-1.92488	0.39981	-2.76853
H	-2.18423	-1.16657	-3.76671

Table V: LDA/BP NLSCF optimized cartesian coordinates for the prone η^4-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**2a**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.09197	-0.09768	0.00000
C	-2.06924	0.35250	0.00000
C	-1.71480	-0.28963	1.21319
C	-1.71480	-0.28963	-1.21319
H	-2.33688	1.41614	0.00000
H	-1.78709	0.24212	2.16666
H	-1.78709	0.24212	-2.16666
H	-1.72217	-1.38840	1.27671
H	-1.72217	-1.38840	-1.27671
C	1.77953	-0.50766	0.72961

C	1.77953	-0.50766	-0.72961
C	1.28057	0.55360	1.48846
C	1.28057	0.55360	-1.48846
H	1.14382	0.42052	2.56563
H	1.14382	0.42052	-2.56563
H	1.27537	1.59390	1.13740
H	1.27537	1.59390	-1.13740
H	1.99382	-1.45994	1.22886
H	1.99382	-1.45994	-1.22886

Table VI: LDA/BP NLSCF optimized cartesian coordinates for the prone η^2-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**2b**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.25026	-0.75714	0.01114
C	-1.84749	-0.91673	1.11355
C	-2.20929	-1.18253	-0.24940
C	-1.86538	-0.17227	-1.15937
C	1.30470	-1.85618	0.71372
C	1.42863	-0.59632	1.30577
C	1.05630	-0.21144	2.67897
C	0.76184	-1.07336	3.67935
H	1.85631	-2.08143	-0.21161
H	0.92158	-2.72620	1.26083
H	1.99271	0.16825	0.74419
H	1.07729	0.86603	2.89048
H	0.52503	-0.70861	4.68432
H	0.78212	-2.16256	3.54856
H	-1.83819	-1.72715	1.85216
H	-1.95630	0.10003	1.52182
H	-2.42003	-2.20436	-0.58877
H	-1.87225	0.88457	-0.85030
H	-1.83133	-0.36762	-2.23840

Table VII: LDA/BP NLSCF optimized cartesian coordinates for the prone transition state of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**2c**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.13820	0.06539	-0.35958
C	-1.21245	-0.12410	1.29822
C	-1.73053	-0.46270	-0.05324
C	-1.70994	0.44412	-1.12744
C	1.35572	-1.23027	-1.30184
C	2.10559	-0.39969	-0.42461
C	1.65308	-0.11326	0.90515
C	0.55330	-0.76118	1.64534
H	1.56596	-1.18412	-2.37643
H	0.88931	-2.16486	-0.95824
H	2.87507	0.26699	-0.83254
H	2.10677	0.76665	1.38059
H	0.56707	-0.50072	2.71209
H	0.42297	-1.83976	1.48673
H	-1.25829	0.94001	1.57944
H	-1.63017	-0.75027	2.09630
H	-2.00425	-1.50893	-0.24163
H	-1.67943	1.53272	-0.96093

H	-2.04648	0.12443	-2.11868

Table VIII: LDA/BP NLSCF optimized cartesian coordinates for the prone product of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**2d**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.34806	0.18425	0.03340
C	-0.78692	-0.69066	2.49285
C	-1.25042	-0.63681	1.04179
C	-1.65055	0.51571	0.36620
C	2.19225	-0.74491	-0.31193
C	2.27449	0.29307	0.62437
C	1.32825	0.32698	1.71656
C	0.76708	-0.81473	2.53861
H	2.69041	-0.63929	-1.28315
H	1.86799	-1.75928	-0.04172
H	2.80981	1.21659	0.36979
H	1.18480	1.32430	2.16353
H	1.12323	-0.71465	3.58154
H	1.10122	-1.79708	2.16689
H	-1.09641	0.22639	3.02352
H	-1.24792	-1.55076	3.00483
H	-1.38835	-1.60414	0.53104
H	-1.76207	1.47884	0.88270
H	-2.13921	0.43819	-0.61581

Table IX: LDA/BP NLSCF optimized cartesian coordinates for the supine η^4-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**3a**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.27028	-0.62284	0.04738
C	-1.21394	-0.55156	1.57205
C	-1.60898	-1.36983	0.48928
C	-1.69386	-0.77291	-0.78815
C	2.05361	-1.00268	1.23262
C	1.41160	-2.17442	0.80765
C	1.14947	-2.40892	-0.59590
C	1.51302	-1.46660	-1.56392
C	0.56089	1.33923	-0.99243
C	0.84334	1.52374	0.34438
H	-1.50449	0.50354	1.58984
H	-0.97281	-0.99897	2.54265
H	-1.60739	-2.46226	0.59233
H	2.07835	-0.75534	2.29830
H	2.81367	-0.51568	0.61530
H	0.94057	-2.83943	1.54057
H	0.49652	-3.24798	-0.86060
H	1.13166	-1.56710	-2.58396
H	2.39915	-0.83816	-1.44474
H	-1.82523	-1.38346	-1.68826
H	-2.00545	0.27309	-0.86819
H	-0.42001	1.58488	-1.40897
H	1.36233	1.22523	-1.72669
H	1.87698	1.57050	0.70095
H	0.08669	1.90093	1.03827

Table X: LDA/BP NLSCF optimized cartesian coordinates for the supine η^2-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**3b**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.11432	-0.08803	0.03990
C	-1.51398	-0.22121	1.53859
C	-2.07566	-0.70053	0.33598
C	-2.01907	0.15577	-0.78291
C	1.32181	-0.02608	1.59664
C	1.56173	-1.19647	0.87521
C	1.12639	-2.55978	1.21229
C	0.81703	-2.99549	2.45689
C	0.58589	-0.07886	-2.03124
C	1.12899	0.96433	-1.30415
H	-1.57047	0.85103	1.77817
H	-1.36894	-0.90071	2.38431
H	-2.25866	-1.77391	0.20065
H	0.82881	-0.05517	2.57337
H	1.91075	0.87499	1.39359
H	2.26229	-1.14122	0.03077
H	1.14241	-3.28432	0.38636
H	0.86498	-2.34034	3.33611
H	0.55644	-4.04424	2.63700
H	-0.26178	0.08222	-2.70225
H	1.11748	-1.03181	-2.15201
H	2.14333	0.90375	-0.89550
H	0.68711	1.96941	-1.34945
H	-2.29464	-0.21583	-1.77416
H	-2.08507	1.24551	-0.64492

Table XI: LDA/BP NLSCF optimized cartesian coordinates for the supine transition state of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**3c**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.18554	0.01789	-0.23915
C	-1.48674	-0.20387	1.24933
C	-1.89947	-0.59312	-0.11113
C	-2.03201	0.27141	-1.16832
C	2.16892	-0.41315	-0.60249
C	1.44290	-1.62889	-0.57192
C	0.60923	-1.90309	0.53825
C	0.44210	-1.04937	1.70547
C	0.61000	1.91460	-1.16552
C	0.51701	2.04622	0.21376
H	-2.05333	-1.66301	-0.29815
H	2.64055	-0.01922	0.30659
H	2.65296	-0.11908	-1.54005
H	1.36153	-2.26436	-1.46087
H	-0.04987	-2.77678	0.46236
H	-1.56810	0.85135	1.52954
H	-1.86672	-0.85930	2.03698
H	1.23437	-0.34395	1.98418
H	0.00534	-1.52965	2.58450
H	-2.31797	-0.09735	-2.15917
H	-2.05755	1.35497	-1.01680
H	1.41688	2.08506	0.83876

H	-0.39858	2.43754	0.67156
H	-0.22637	2.16432	-1.82305
H	1.58208	1.84885	-1.66161

Table XII: LDA/BP NLSCF optimized cartesian coordinates for the supine product of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**3d**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.33581	0.31515	-0.45210
C	-1.86486	-0.94300	1.27851
C	-1.80661	-0.40784	-0.15707
C	-1.72070	0.92776	-0.49392
C	2.15596	-0.02392	0.35100
C	1.59251	-1.26859	-0.02649
C	0.31421	-1.65146	0.43469
C	-0.41546	-1.28708	1.71900
C	1.06966	1.53825	-1.95728
C	0.84425	2.34008	-0.84546
H	-1.98025	-1.12714	-0.96878
H	1.97411	0.40605	1.34646
H	3.07061	0.32176	-0.14476
H	2.00224	-1.79507	-0.89770
H	-0.14649	-2.48362	-0.11547
H	-2.32598	-0.20776	1.95742
H	-2.50233	-1.84332	1.29143
H	0.04158	-0.42089	2.22598
H	-0.37262	-2.13200	2.43231
H	-1.89098	1.25159	-1.52816
H	-1.77618	1.70306	0.28172
H	1.66285	2.60601	-0.16649
H	-0.06186	2.94749	-0.75973
H	0.32813	1.46473	-2.76236
H	2.07260	1.16991	-2.20219

Table XIII: LDA/BP NLSCF optimized cartesian coordinates for the prone η^4-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**4a**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.12053	-0.45106	-0.03130
C	-1.42891	-0.77055	1.50069
C	-1.81601	-1.07691	0.18290
C	-1.71429	-0.06959	-0.82624
C	1.27342	-1.69161	1.40308
C	2.02353	-1.19756	0.33457
C	1.69126	-1.49136	-1.05363
C	0.58569	-2.25990	-1.38362
C	0.84436	1.46523	-0.79985
C	0.53792	1.58990	0.54399
H	1.47515	-1.33084	2.41598
H	0.70377	-2.62312	1.32912
H	2.81168	-0.46170	0.52754
H	2.24330	-0.96493	-1.83921
H	0.24623	-2.30378	-2.42359
H	0.17942	-3.01766	-0.70750
H	-1.47637	0.25228	1.88504
H	-1.37175	-1.56192	2.25398

H	-1.99048	-2.12095	-0.10039
H	-1.92419	0.97356	-0.56769
H	-1.88362	-0.33790	-1.87422
H	0.14677	1.78509	-1.58035
H	1.87945	1.31561	-1.12362
H	-0.41425	2.02594	0.86483
H	1.31863	1.54203	1.31163

Table XIV: LDA/BP NLSCF optimized cartesian coordinates for the prone η^2-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system **(4b)**

atom	x coordinate	y coordinate	z coordinate
Ni	-0.11703	-0.46133	-0.24695
C	-1.60190	-0.88052	1.08560
C	-2.02614	-1.22781	-0.21595
C	-2.00648	-0.20310	-1.18887
C	1.15646	-1.80498	0.68380
C	1.46638	-0.62576	1.36712
C	1.01623	-0.23582	2.71253
C	0.67746	-1.10027	3.69588
C	0.37944	0.32144	-2.25761
C	1.40949	0.49937	-1.35457
H	1.78409	-2.13716	-0.15247
H	0.54940	-2.58707	1.15385
H	2.25287	0.01685	0.95410
H	1.05833	0.83844	2.93931
H	0.41188	-0.73881	4.69542
H	0.70698	-2.18798	3.55596
H	-1.46429	-1.64555	1.85679
H	-1.75241	0.14390	1.46156
H	-2.10259	-2.28089	-0.51712
H	-2.21479	0.83476	-0.89098
H	-2.17719	-0.44149	-2.24386
H	-0.28501	1.15219	-2.51471
H	0.35184	-0.55220	-2.92018
H	1.55371	1.47203	-0.86595
H	2.25829	-0.19281	-1.33870

Table XV: LDA/BP NLSCF optimized cartesian coordinates for the prone transition state of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system **(4c)**

atom	x coordinate	y coordinate	z coordinate
Ni	0.12086	-0.01276	-0.27768
C	-1.36428	-0.12734	1.37168
C	-1.85559	-0.40778	0.02805
C	-1.77967	0.52264	-1.01941
C	0.47928	-2.16860	-0.92525
C	1.61208	-1.50229	-0.46759
C	1.59968	-0.80201	0.79569
C	0.50870	-0.94917	1.74311
C	1.09567	1.49898	-1.35874
C	0.77528	1.98663	-0.09264
H	0.41848	-2.49633	-1.96782
H	-0.23289	-2.62868	-0.23479
H	2.45504	-1.32272	-1.14327
H	2.45365	-0.16865	1.05528

H	0.64503	-0.44037	2.70381
H	0.08911	-1.95638	1.83178
H	-1.29800	0.92249	1.68085
H	-1.74908	-0.78070	2.16186
H	-2.19780	-1.42483	-0.19276
H	-1.77924	1.59884	-0.82474
H	-2.08589	0.21641	-2.02541
H	0.47421	1.72388	-2.23162
H	2.10958	1.14637	-1.57986
H	-0.10186	2.62456	0.06240
H	1.53632	2.03727	0.69442

Table XVI: LDA/BP NLSCF optimized cartesian coordinates for the prone product of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**4d**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.27729	0.51467	-0.16761
C	-1.57458	-1.63094	0.72234
C	-1.76109	-0.31080	-0.02135
C	-1.73921	0.93074	0.58299
C	2.20732	-0.12554	-0.24136
C	1.79692	-0.04051	1.11141
C	0.59189	-0.65311	1.52547
C	-0.06892	-1.91456	0.99958
C	0.60782	2.13400	-1.50864
C	0.13751	1.05712	-2.23370
H	3.01451	0.51688	-0.60795
H	2.04022	-1.04260	-0.82366
H	2.21159	0.75168	1.74664
H	0.18503	-0.28969	2.47968
H	0.01867	-2.70205	1.77180
H	0.43016	-2.30338	0.09745
H	-2.12000	-1.57965	1.68117
H	-2.00456	-2.46216	0.14005
H	-2.05549	-0.37460	-1.07694
H	-1.67729	1.03580	1.67282
H	-2.02083	1.83227	0.02735
H	1.67735	2.36057	-1.44395
H	-0.07716	2.91316	-1.15457
H	0.82197	0.38267	-2.76292
H	-0.91912	1.00003	-2.51608

Table XVII: LDA optimized cartesian coordinates for the supine η^4-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**1a**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.08140	0.00000	0.00000
C	-1.99817	-0.47825	0.00000
C	-1.64029	0.16458	1.20195
C	-1.64029	0.16458	-1.20195
H	-2.23271	-1.55383	0.00000
H	-1.69056	-0.37575	2.15766
H	-1.69056	-0.37575	-2.15766
H	-1.67411	1.26875	1.26985
H	-1.67411	1.26875	-1.26985
C	1.66499	-0.65766	0.72261

C	1.66499	-0.65766	-0.72261
C	1.26801	0.44401	1.46878
C	1.26801	0.44401	-1.46878
H	1.08711	0.32041	2.54438
H	1.08711	0.32041	-2.54438
H	1.40400	1.48687	1.13043
H	1.40400	1.48687	-1.13043
H	1.74305	-1.63562	1.22075
H	1.74305	-1.63562	-1.22076

Table XVIII: LDA optimized cartesian coordinates for the supine η^2-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)]^+$ system **(1b)**

atom	x coordinate	y coordinate	z coordinate
Ni	-0.19566	-0.21302	0.29482
C	-1.60409	-0.16970	1.57342
C	-2.09890	-0.71360	0.34850
C	-1.87878	0.08481	-0.77121
C	1.29840	0.09799	1.56782
C	1.47122	-1.11227	0.90125
C	1.18352	-2.45488	1.38462
C	0.95658	-2.76703	2.67364
H	-1.72640	0.90726	1.79229
H	-1.45765	-0.83237	2.43936
H	-2.32468	-1.78678	0.25844
H	0.95187	0.14271	2.61206
H	1.79505	1.00615	1.18807
H	1.99707	-1.07099	-0.07835
H	1.21377	-3.25482	0.62874
H	0.98394	-2.00889	3.47042
H	0.77897	-3.80578	2.98060
H	-1.94254	-0.33341	-1.78734
H	-1.89741	1.18663	-0.69015

Table XIX: LDA optimized cartesian coordinates for the supine transition state of the $[Ni(C_3H_5)(C_4H_6)]^+$ system **(1c)**

atom	x coordinate	y coordinate	z coordinate
Ni	0.03952	-1.23698	-1.72543
C	-1.32165	-1.25265	0.07994
C	-1.82313	-1.37412	-1.33335
C	-1.81192	-0.35635	-2.26637
C	1.21478	0.31440	-2.06109
C	1.93199	-0.77069	-1.51037
C	1.37420	-1.42273	-0.37758
C	0.28321	-0.86782	0.46420
H	-2.18859	-2.36659	-1.65374
H	0.76248	1.08711	-1.41708
H	1.42400	0.63166	-3.09257
H	2.73706	-1.26892	-2.06849
H	1.76878	-2.42229	-0.12741
H	-1.81922	-0.40041	0.57901
H	-1.54596	-2.17839	0.63123
H	0.33150	0.23322	0.51319
H	0.35443	-1.27468	1.49047
H	-1.65305	0.69625	-1.98719

H	-2.20202	-0.54036	-3.27692

Table XX: LDA optimized cartesian coordinates for the supine product of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**1d**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.14110	-0.91833	-2.44091
C	-1.45457	-0.96368	-0.27718
C	-1.68657	-1.47218	-1.66642
C	-1.81071	-0.71596	-2.81237
C	1.69178	0.04778	-1.71657
C	1.83946	-1.33641	-1.55928
C	0.72940	-1.98722	-0.93732
C	-0.09466	-1.52256	0.23424
H	-1.81846	-2.56528	-1.76436
H	1.19965	0.67625	-0.95424
H	2.31184	0.58055	-2.45664
H	2.56777	-1.91139	-2.14883
H	0.61431	-3.05425	-1.20367
H	-1.43389	0.14299	-0.27499
H	-2.28122	-1.28513	0.38696
H	0.43471	-0.76022	0.83460
H	-0.26464	-2.39368	0.89592
H	-1.85175	0.38972	-2.74629
H	-2.11767	-1.17434	-3.76416

Table XXI: LDA optimized cartesian coordinates for the prone η^4-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**2a**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.07334	-0.11313	0.00000
C	-2.00361	0.37526	0.00000
C	-1.62975	-0.26237	1.19953
C	-1.62975	-0.26237	-1.19953
H	-2.29284	1.43807	0.00000
H	-1.70760	0.25800	2.16236
H	-1.70760	0.25800	-2.16236
H	-1.61221	-1.36693	1.25014
H	-1.61221	-1.36693	-1.25014
C	1.73958	-0.51729	0.72210
C	1.73958	-0.51729	-0.72210
C	1.19380	0.53085	1.45770
C	1.19380	0.53085	-1.45770
H	1.05058	0.40049	2.53685
H	1.05058	0.40049	-2.53685
H	1.18820	1.57455	1.10442
H	1.18820	1.57455	-1.10442
H	1.96232	-1.46748	1.23050
H	1.96232	-1.46748	-1.23050

Table XXII: LDA optimized cartesian coordinates for the prone η^2-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**2b**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.24576	-0.74039	0.02878
C	-1.78891	-0.92723	1.11966
C	-2.16746	-1.19418	-0.22898

C	-1.79611	-0.19238	-1.12174
C	1.22523	-1.84277	0.71029
C	1.34356	-0.57942	1.28331
C	1.00528	-0.20089	2.65238
C	0.74730	-1.07156	3.64395
H	1.76806	-2.07361	-0.22541
H	0.84802	-2.71525	1.26810
H	1.91011	0.18349	0.71128
H	1.02825	0.87695	2.87767
H	0.53652	-0.72191	4.66442
H	0.78539	-2.16225	3.49509
H	-1.74819	-1.73302	1.87064
H	-1.90470	0.09368	1.53068
H	-2.40693	-2.21271	-0.56982
H	-1.77779	0.86553	-0.79821
H	-1.74587	-0.37708	-2.20509

Table XXIII: LDA optimized cartesian coordinates for the prone transition state of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**2c**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.12559	0.03916	-0.30602
C	-1.17615	-0.11905	1.29066
C	-1.69809	-0.48788	-0.03783
C	-1.63350	0.38955	-1.12545
C	1.29381	-1.17554	-1.29528
C	2.06173	-0.36907	-0.42364
C	1.63154	-0.11241	0.90636
C	0.52208	-0.76202	1.61560
H	1.47942	-1.10649	-2.37635
H	0.84363	-2.12772	-0.96225
H	2.83848	0.29410	-0.83153
H	2.09639	0.75167	1.40549
H	0.54974	-0.53805	2.69530
H	0.39806	-1.84411	1.44114
H	-1.21092	0.96006	1.53564
H	-1.61776	-0.69632	2.11778
H	-1.99339	-1.53619	-0.20228
H	-1.59497	1.48583	-0.97831
H	-1.95449	0.05483	-2.12035

Table XXIV: LDA optimized cartesian coordinates for the prone product of the $[Ni(C_3H_5)(C_4H_6)]^+$ system (**2d**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.35125	0.17314	0.06881
C	-0.76750	-0.68744	2.48233
C	-1.20198	-0.64231	1.04257
C	-1.58092	0.50510	0.36095
C	2.12925	-0.73329	-0.29176
C	2.23587	0.30089	0.63382
C	1.30453	0.32089	1.72361
C	0.76452	-0.81507	2.52753
H	2.60619	-0.63252	-1.27846
H	1.80585	-1.75050	-0.01171
H	2.76321	1.22883	0.36464
H	1.12376	1.32038	2.16420

H	1.12808	-0.73282	3.57364
H	1.09617	-1.79569	2.13842
H	-1.07716	0.24125	3.00057
H	-1.23928	-1.53975	3.00498
H	-1.33291	-1.61598	0.53396
H	-1.68611	1.47321	0.87926
H	-2.05705	0.43369	-0.63237

Table XXV: LDA optimized cartesian coordinates for the supine η^4-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**3a**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.28444	-0.61379	0.03939
C	-1.13551	-0.54173	1.53840
C	-1.53781	-1.36509	0.47480
C	-1.60940	-0.75767	-0.78836
C	1.98213	-0.95307	1.19360
C	1.35471	-2.14399	0.80832
C	1.09395	-2.37544	-0.58038
C	1.45255	-1.39949	-1.51464
C	0.54309	1.22233	-0.97482
C	0.81921	1.40722	0.36433
H	-1.44016	0.51337	1.54862
H	-0.88172	-0.97511	2.51592
H	-1.52476	-2.46100	0.57258
H	2.01557	-0.67416	2.25551
H	2.76479	-0.50494	0.56549
H	0.89297	-2.80023	1.55944
H	0.44486	-3.21387	-0.86905
H	1.08398	-1.47626	-2.54649
H	2.36794	-0.80570	-1.38559
H	-1.73605	-1.35671	-1.70065
H	-1.93939	0.28773	-0.85396
H	-0.43434	1.49445	-1.39170
H	1.35243	1.14061	-1.71028
H	1.85532	1.48556	0.71557
H	0.06677	1.80996	1.05392

Table XXVI: LDA optimized cartesian coordinates for the supine η^2-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**3b**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.04353	-0.09309	-0.00373
C	-1.40410	-0.35253	1.43911
C	-1.83552	-0.96154	0.25440
C	-1.88786	-0.13379	-0.88280
C	1.33936	-0.00019	1.48914
C	1.47619	-1.23892	0.86364
C	0.96706	-2.51811	1.33380
C	0.69925	-2.79758	2.62236
C	0.25699	0.39680	-2.00963
C	1.26466	0.86024	-1.18115
H	-1.63109	0.71323	1.62294
H	-1.16665	-0.97058	2.31566
H	-1.84829	-2.05871	0.15846
H	0.83976	0.08149	2.46471

H	2.04532	0.80763	1.25271
H	2.18784	-1.31993	0.02702
H	0.90009	-3.32202	0.58360
H	0.85010	-2.05538	3.42268
H	0.38449	-3.80366	2.93019
H	-0.49274	1.09685	-2.40210
H	0.36856	-0.54790	-2.56420
H	2.23130	0.33942	-1.12248
H	1.26112	1.91157	-0.84510
H	-2.09051	-0.56308	-1.87300
H	-2.18180	0.92278	-0.75697

Table XXVII: LDA optimized cartesian coordinates for the supine transition state of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**3c**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.13276	-0.00367	-0.22355
C	-1.43478	-0.22139	1.23976
C	-1.84220	-0.59269	-0.11456
C	-1.88295	0.28971	-1.16102
C	2.05594	-0.39907	-0.67296
C	1.34818	-1.61373	-0.59901
C	0.57923	-1.86099	0.54871
C	0.46992	-0.95072	1.66667
C	0.64236	1.83184	-1.10057
C	0.41990	1.96129	0.25817
H	-2.02641	-1.65692	-0.32116
H	2.57069	0.00628	0.21367
H	2.50697	-0.12216	-1.63535
H	1.24576	-2.27483	-1.47012
H	-0.08692	-2.73708	0.53865
H	-1.55808	0.82612	1.54666
H	-1.80147	-0.90531	2.01373
H	1.29661	-0.25124	1.86933
H	0.08797	-1.37873	2.60075
H	-2.14801	-0.05140	-2.17078
H	-1.91509	1.37309	-0.98209
H	1.26357	2.02134	0.96210
H	-0.54099	2.34629	0.63034
H	-0.13424	2.06582	-1.83871
H	1.66509	1.82526	-1.49610

Table XXVIII: LDA optimized cartesian coordinates for the supine product of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**3d**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.19581	0.05181	-0.51997
C	-1.55479	-0.38756	1.84466
C	-1.66353	-0.62462	0.34969
C	-1.81714	0.38175	-0.57860
C	2.07034	0.33900	0.00680
C	1.70453	-0.97976	0.32480
C	0.56219	-1.21806	1.10456
C	-0.05824	-0.37635	2.18568
C	0.35541	1.58663	-1.88543
C	0.61151	0.35334	-2.45741

H	-1.80277	-1.66258	0.00789
H	1.89175	1.16924	0.71272
H	2.85819	0.51947	-0.73812
H	2.12006	-1.81219	-0.26278
H	0.18979	-2.25587	1.08348
H	-2.04422	0.55924	2.13476
H	-2.08007	-1.20087	2.37873
H	0.33229	0.65825	2.18694
H	0.17302	-0.80315	3.18175
H	-2.13282	0.15215	-1.60842
H	-1.94489	1.42371	-0.24122
H	1.17967	2.24583	-1.57249
H	-0.62228	2.07146	-2.00666
H	-0.17369	-0.19751	-2.99682
H	1.63964	0.00662	-2.63459

Table XXIX: LDA optimized cartesian coordinates for the prone η^4-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**4a**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.15110	-0.47892	-0.02942
C	-1.36117	-0.78429	1.44094
C	-1.75911	-1.06174	0.12773
C	-1.61357	-0.04310	-0.84931
C	1.26507	-1.62159	1.37688
C	2.01916	-1.14843	0.30511
C	1.64154	-1.45733	-1.05082
C	0.50121	-2.20946	-1.27840
C	0.82144	1.36716	-0.76707
C	0.48468	1.47987	0.56834
H	1.46946	-1.24124	2.38618
H	0.74061	-2.58550	1.32612
H	2.80630	-0.39863	0.47468
H	2.15438	-0.95209	-1.88012
H	0.08352	-2.26060	-2.29262
H	0.18003	-2.99466	-0.58092
H	-1.40737	0.23735	1.83934
H	-1.34177	-1.58787	2.18753
H	-1.97842	-2.09345	-0.17846
H	-1.80222	1.00160	-0.56241
H	-1.77393	-0.27889	-1.90958
H	0.13654	1.69437	-1.56053
H	1.87224	1.25773	-1.06780
H	-0.48689	1.90171	0.86396
H	1.25389	1.47601	1.35340

Table XXX: LDA optimized cartesian coordinates for the prone η^2-butadiene educt of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**4b**)

atom	x coordinate	y coordinate	z coordinate
Ni	-0.07633	-0.46254	-0.21973
C	-1.52705	-0.86560	1.10417
C	-1.93551	-1.22156	-0.18344
C	-1.87868	-0.20726	-1.16064
C	1.14674	-1.78517	0.64644
C	1.42982	-0.59480	1.30814

C	0.95115	-0.21390	2.63052
C	0.60133	-1.09094	3.58633
C	0.28698	0.29089	-2.14412
C	1.36320	0.43909	-1.28776
C	1.79520	-2.13342	-0.17097
H	0.53553	-2.56287	1.12931
H	2.24383	0.03395	0.91699
H	0.97090	0.86229	2.86876
H	0.30267	-0.75113	4.58722
H	0.66169	-2.17905	3.42631
H	-1.39193	-1.61509	1.89581
H	-1.65257	0.17215	1.46411
H	-2.03103	-2.27922	-0.47431
H	-2.11175	0.82965	-0.86261
H	-2.07919	-0.44848	-2.21276
H	-0.32826	1.16132	-2.40600
H	0.24145	-0.55964	-2.83993
H	1.55512	1.41590	-0.81581
H	2.21168	-0.25914	-1.33203

Table XXXI: LDA optimized cartesian coordinates for the prone transition state of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**4c**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.11789	-0.05359	-0.23574
C	-1.33819	-0.09127	1.32618
C	-1.81074	-0.41597	0.00510
C	-1.66210	0.47306	-1.06610
C	0.39230	-2.07359	-0.88507
C	1.57676	-1.45516	-0.50419
C	1.62899	-0.78249	0.75767
C	0.54032	-0.90404	1.69140
C	1.04849	1.43279	-1.27613
C	0.71083	1.88891	-0.00990
H	0.24356	-2.37841	-1.92933
H	-0.23969	-2.58177	-0.14406
H	2.38388	-1.28394	-1.22937
H	2.48890	-0.13969	0.99034
H	0.66802	-0.37824	2.64796
H	0.10896	-1.91010	1.79136
H	-1.28185	0.97004	1.61003
H	-1.69495	-0.73481	2.14146
H	-2.16091	-1.43925	-0.19185
H	-1.67762	1.55883	-0.90314
H	-1.92340	0.13540	-2.07839
H	0.43964	1.67903	-2.15631
H	2.07479	1.10313	-1.49198
H	-0.17555	2.52113	0.14415
H	1.47033	1.94945	0.78331

Table XXXII: LDA optimized cartesian coordinates for the prone product of the $[Ni(C_3H_5)(C_4H_6)(C_2H_4)]^+$ system (**4d**)

atom	x coordinate	y coordinate	z coordinate
Ni	0.17365	0.31883	-0.43947
C	-1.15322	-0.94098	1.82809

C	-1.61738	-0.30359	0.54443
C	-1.64588	1.05107	0.31085
C	2.05581	-0.25170	-0.70412
C	1.96656	0.49840	0.48271
C	0.96933	0.18699	1.41855
C	0.36353	-1.14710	1.74866
C	0.10891	1.03443	-2.34387
C	-0.57230	-0.16078	-2.26995
H	2.69859	0.09674	-1.52395
H	1.83806	-1.33516	-0.71309
H	2.43841	1.49239	0.52429
H	0.73340	0.97629	2.15413
H	0.76054	-1.48694	2.72760
H	0.61943	-1.93212	1.00959
H	-1.38889	-0.27305	2.68065
H	-1.67189	-1.90138	2.00463
H	-2.04971	-0.97569	-0.21404
H	-1.43644	1.77511	1.11162
H	-2.14118	1.45466	-0.58535
H	1.12064	1.09537	-2.76111
H	-0.40969	1.99855	-2.22337
H	-0.09706	-1.10158	-2.58891
H	-1.66715	-0.17372	-2.18097