Electronic Supplementary Material (ESI) for RSC Advances.

Supporting Information

Theoretical Study on the Reaction Mechanism of "Ligandless" Ni-Catalyzed Hydrodesulfurization of Aryl Sulfide

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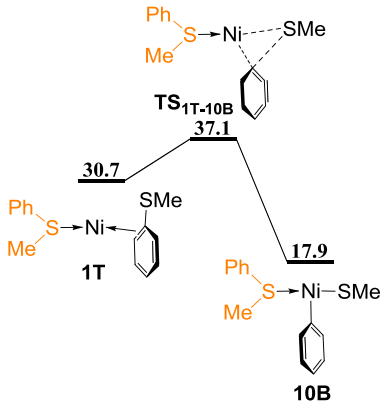

Figure S1. Energy profile of oxidative addition process from complex **1T** (values are given in kcal/mol).

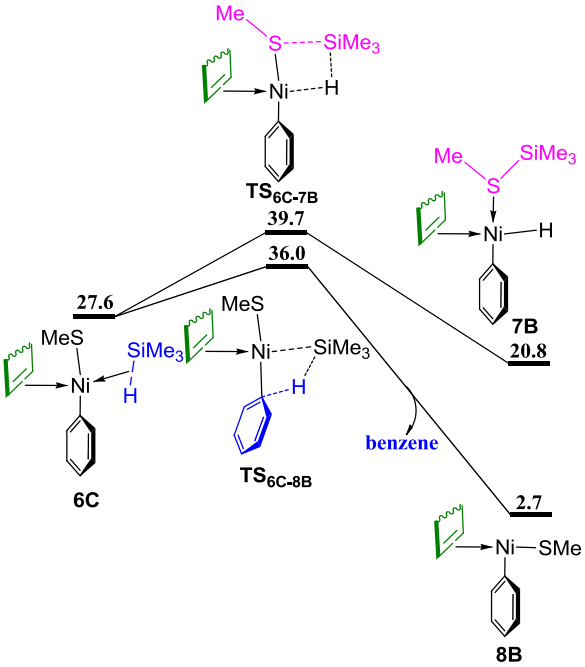

Figure S2. Energy profiles of σ-CAM process from complex **6C** with $HSiMe_3$ (values are given in kcal/mol).

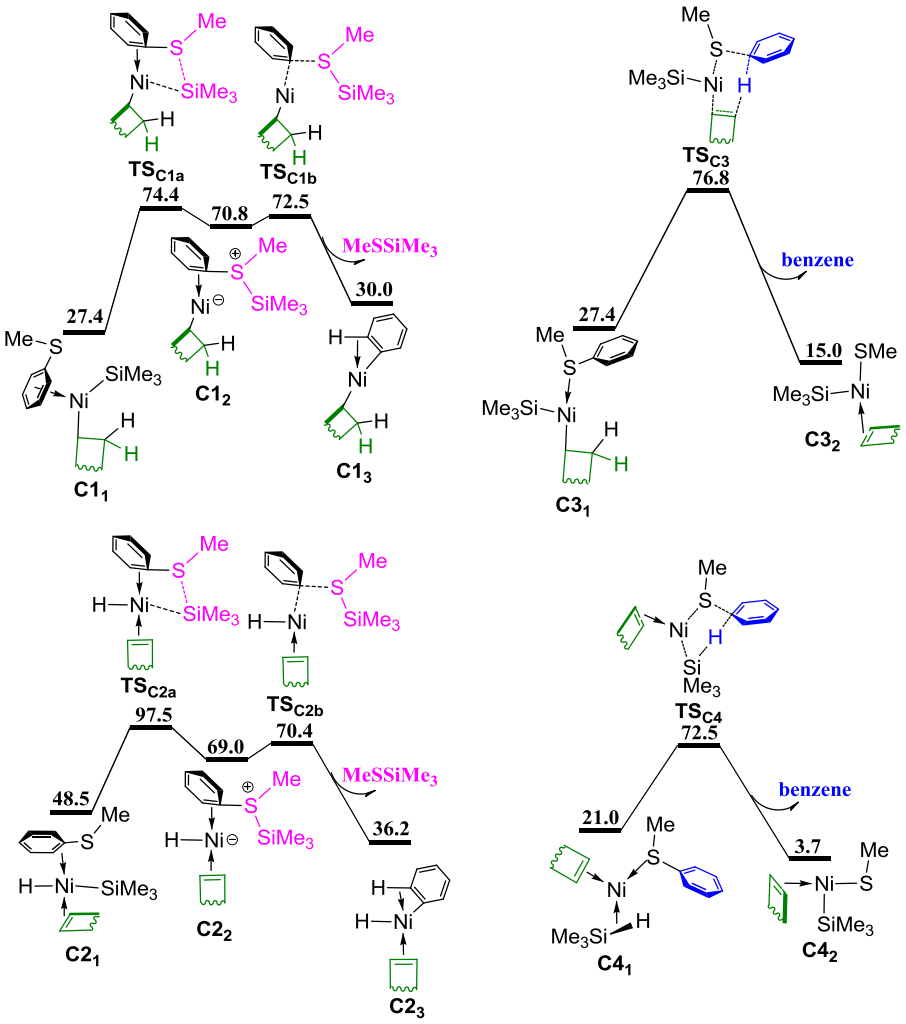

Figure S3. Energy profile of COD coordianted metathesis or quasi-metathesis process from various Ni-hydride species (values are given in kcal/mol).

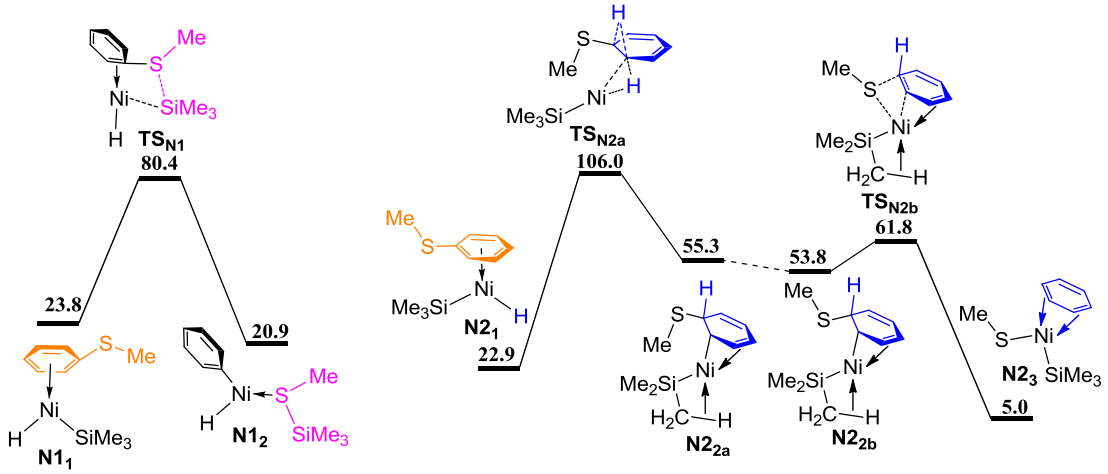

Figure S4. Energy profile of metathesis or quasi-metathesis process from various Ni-hydride species on "ligandless" pathways (values are given in kcal/mol).

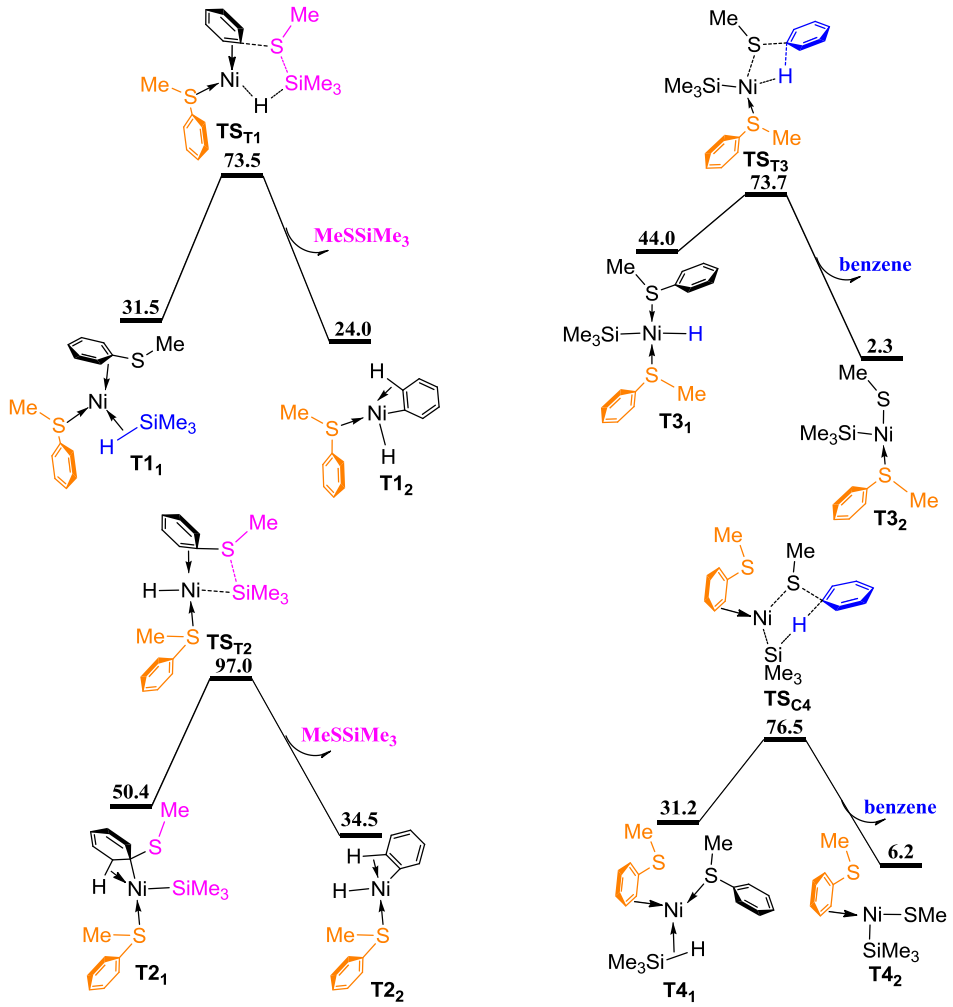

Figure S5. Energy profile of metathesis or quasi-metathesis process from various Ni-hydride species on PhSMe-coordianted pathways (values are given in kcal/mol).

Table S1. The Gibbs free energy singlet-triplet gap between complex **11** and **11³** using different post-HF and DFT methods.

Method	basis set	G(**11**)-G(**11³**)
CASMP2(12,11)$^{\alpha}$	def2-TZVP [1]	4.7
CCSD(TQ)*$^{\beta,2}$	def2-TZVP	4.3
CCSD(T)	def2-TZVP	1.2
QCISD(T)	def2-TZVP	-1.4
ωB97XD	def2-TZVP	6.4
ωB97XD	6-311++g(d,p)	6.5
ωB97XD	def2-QZVPPD	6.2
B3LYP* [3]	def2-TZVP	0.4
PBE0	def2-TZVP	8.3
PBE	def2-TZVP	-7.4
M06	def2-TZVP	-1.0

$^{\alpha}$including 12 electrons of Ni and S along with 11 orbitals, $^{\beta}$ see ref 2 ,estimate by the E5TT,E5TQ2 and E5QQ value using small model($HSNiCH_3$) calculated by QCISD(TQ)/def2-TZVP

$$E(CCSD(TQ)) = E(CCSD(T)) + 0.5 * E5TQ1 + E5TT + E5TQ2 + E5QQ$$

$$= E(CCSD(T)) + E(CCSD(T)) - E(QCISD(T)) + E5TT + E5TQ2 + E5QQ$$

$$\approx 2 * E(CCSD(T)) - E(QCISD(T)) + E5TT_{small\text{-}model} + E5TQ2_{small\text{-}model} + E5QQ_{small\text{-}model}$$

$$= 2 * E(CCSD(T)) - E(QCISD(T)) + E_{corr}(TQ^*)$$

$$= E(CCSD(TQ)^*)$$

For the gap between **11** and **11^3** is evaluated by CCSD(TQ)* , the value of $E_{corr}(TQ^*)$ is only 0.8 kcal/mol, contributing little to the overall result.

References

1 (a) F. Weigend and R. Ahlrichs, *Phys. Chem. Chem.* , *Phys.* **2005**, *7*, 3297−3305. (b) F. Weigend, *Phys. Chem. Chem. Phys.* , **2006**, *8*, 1057−1065.

2 K. Raghavachari, J. A. Pople, E. S. Replogle and M. Head-Gordon, *J. Phys. Chem.*, **1990**, *94*, 5579−5586.

3 O. Salomon, M. Reiher and B. A. Hess, *J. Chem. Phys.* , **2002**, *117*, 4729−4737.

Calculated Cartesian coordinates for the involved species in the paper

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1 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	5.9790478715	1.2368018013	2.5214546555
C	6.5803553974	2.8360843243	3.7739513264
C	7.6954665486	2.3022904654	3.1390691399
C	8.3570214462	2.8576485566	1.892706607
C	7.3409403484	3.3295614489	0.8284124636
C	6.0851379517	2.4640987553	0.7980648232
C	4.9015726383	2.7243526944	1.478476983
C	4.6660556323	3.872602263	2.4410122702
C	5.8631246208	4.1249762096	3.3848806799
C	7.1770255526	-0.4904696097	2.3059755672
C	6.1466447268	-0.5370070329	1.3745911231
C	4.876943222	-1.3748687321	1.4886660027
C	3.7013480906	-0.58409119	2.1055491087
C	4.1441158519	0.4094609193	3.1621782166
C	5.1064688007	0.1821939397	4.138716767
C	5.8374481665	-1.1343386443	4.3820333059
C	7.1943938992	-1.2001734297	3.6459045692
H	6.424345117	2.5263955957	4.8043466427
H	8.3293486149	1.6442737277	3.7319111193
H	8.9816524766	2.0654963475	1.4601356525
H	9.0492054938	3.6761781343	2.1503547074
H	7.0720939131	4.3779152439	0.993419292
H	7.8158568551	3.2999767518	-0.159728178
H	6.0025417331	1.8191279781	-0.0731862309
H	3.9931582146	2.2849569504	1.0686887852
H	3.7825032809	3.6302572743	3.0456851695
H	4.4092829198	4.7939924073	1.8933849237
H	6.5693911284	4.8262835368	2.9289052488
H	5.504310184	4.6197805216	4.2954895196
H	8.159189201	-0.1987358329	1.9365490137
H	6.4085777625	-0.2509367526	0.3589750551
H	4.5905710974	-1.7222257492	0.4886315589
H	5.0750176113	-2.2819880755	2.0687900342
H	3.1925984812	-0.0259250259	1.3090469493
H	2.9465736515	-1.2765275936	2.5133327774
H	3.4360941342	1.2156650338	3.3491140469
H	5.0838317776	0.8509482502	4.9955963669
H	5.2022797254	-1.9772577881	4.0911087083
H	6.0068423953	-1.2520764532	5.4591708007
H	7.9605483016	-0.7234844812	4.2708520551
H	7.5153751639	-2.2482707035	3.5278823726

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3 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.3329594936	0.2241579018	0.3157097175
C	-2.3967174247	0.1384331095	0.6614821151
C	-1.7911873947	0.8576159391	1.6730731477
C	-1.6437745964	2.3644046491	1.7438983988
C	-1.3065162406	3.0274607151	0.380492195
C	-0.3734218071	2.180894893	-0.4716327637
C	-0.7560994874	1.2769578865	-1.4417718448
C	-2.1743218477	0.8655213434	-1.782296419
C	-3.1081136697	0.7248682126	-0.5475203135

H	-2.5865368668	-0.9173988652	0.8497842185
H	-1.5854745057	0.3327766987	2.6054773077
H	-0.8364936228	2.5859662097	2.4530268883
H	-2.5496637493	2.8264426395	2.1663854295
H	-2.2245128965	3.2493576601	-0.1715908223
H	-0.8303692076	3.9961591425	0.5713795963
H	0.6686962594	2.499056018	-0.4830965523
H	-0.0034439376	0.9680710718	-2.1646261356
H	-2.1220125832	-0.1019204579	-2.2971061867
H	-2.6215516137	1.5671754473	-2.5034747167
H	-3.5508841916	1.6923773122	-0.2937557963
H	-3.9463762715	0.0720101567	-0.8171071306
S	2.7047702994	0.3959392827	0.2343367471
C	4.1162584877	-0.7272270363	0.5804976476
H	5.0019482087	-0.0977634107	0.7087989287
H	3.9439299641	-1.2977410585	1.4971851254
H	4.2799134836	-1.4135118126	-0.2546535814
C	1.3453725118	-0.7778331183	0.0061044709
C	1.3535898296	-1.5885032157	-1.1895804006
C	0.6169991143	-1.2994752334	1.1598781269
C	0.6901224049	-2.788683252	-1.2512959308
H	1.910824155	-1.2253007422	-2.0501029827
C	0.0213448559	-2.6051522563	1.071704381
H	0.8940205806	-0.9484139494	2.1549961914
C	0.0222911672	-3.3128146348	-0.1039499914
H	0.7038543148	-3.3654744196	-2.1729961366
H	-0.4272190634	-3.033856563	1.9659597727
H	-0.4480031653	-4.2912612631	-0.1571907011

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$TS_{3\text{-}4}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.3611951301	0.3018878809	0.265038665
C	2.0711560556	0.334453743	-1.0778532422
C	2.436160529	0.7700537441	0.1745389583
C	3.0011465292	-0.0736607387	1.300921613
C	2.3707131892	-1.4881764113	1.4342337288
C	0.8769443067	-1.515463568	1.1370334805
C	0.3136912	-1.7424504699	-0.111325049
C	1.040685264	-1.977565042	-1.42102862
C	2.2772373234	-1.0692996208	-1.6228237168
H	1.8406020517	1.1014261786	-1.8180213267
H	2.5080746491	1.8443005385	0.333269133
H	2.8291391737	0.4764216808	2.2335278223
H	4.0937468667	-0.1650795143	1.197922105
H	2.8945236266	-2.1970924279	0.7848982099
H	2.5376233937	-1.8423215699	2.4580524883
H	0.2252712903	-1.6414980136	2.0006025319
H	-0.7357967036	-2.0294415301	-0.1262855508
H	0.3255491244	-1.7829029229	-2.2302624671
H	1.3317187444	-3.0351592167	-1.5247998285
H	3.1610129382	-1.5187908355	-1.1601916336
H	2.5020246565	-1.0041451413	-2.6941296808
S	-0.3469769329	2.0413452861	1.4760830494
C	-0.3374814629	3.5098173254	0.3829399665
H	-0.462172334	4.3947942654	1.0124696777
H	0.5929620624	3.5955141792	-0.1871579186
H	-1.1841935688	3.4494747045	-0.3084727889
C	-1.4973302125	0.6155765188	0.5243262633

C	-2.4235054833	-0.095219873	1.3324515457
C	-1.8579942448	0.8972559074	-0.8189816152
C	-3.5928484858	-0.5939157411	0.7830549426
H	-2.1997031722	-0.2639265032	2.3825986897
C	-3.0355243659	0.364220342	-1.3603607057
H	-1.2306330877	1.5296133766	-1.4427358152
C	-3.9066381834	-0.3825025295	-0.5733457935
H	-4.2785271886	-1.1560584203	1.4134890074
H	-3.2765136145	0.5623358295	-2.4027164476
H	-4.830526674	-0.7731111107	-0.9896168183

37 (charge = 0, singlet)

4 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.1014636184	0.4303321458	-0.0622796319
C	1.8950917557	-0.362154752	0.7128745831
C	1.8632489954	-0.4953264408	-0.6649911043
C	2.5312597299	0.3908843249	-1.6940943433
C	2.5325834155	1.8917043903	-1.324664247
C	1.2318943909	2.328687012	-0.6813258794
C	0.967328701	2.3819417574	0.6572720327
C	1.8655910486	1.9480180231	1.7946084779
C	2.6872164014	0.6733766287	1.4978120326
H	1.5541946682	-1.2220066187	1.2844969064
H	1.5312366774	-1.4558889605	-1.0512264475
H	1.9975945161	0.2590193762	-2.6433555286
H	3.5604402452	0.0444284892	-1.8768738274
H	3.3748774908	2.1243042416	-0.6676032305
H	2.6864426012	2.4805795912	-2.2358188298
H	0.502560726	2.7926982294	-1.3408626595
H	0.0697338323	2.9156426101	0.9572498788
H	1.227262887	1.7649989739	2.6668556629
H	2.5340111709	2.7749127643	2.0790673397
H	3.6098759115	0.9248976938	0.966443341
H	3.0006594725	0.2280863415	2.4486981123
S	-1.7978330461	1.4618045449	-0.3237880353
C	-0.8132523648	-1.2296864905	0.0380715267
C	-1.1635575811	-1.7637621975	1.2886455997
C	-1.0796549764	-2.00639852	-1.1008655764
C	-1.7535319508	-3.028014617	1.3980975207
H	-0.990761059	-1.1882529977	2.1963028069
C	-1.6680247898	-3.2711605835	-0.9957068321
H	-0.8408717098	-1.6212075778	-2.0907023257
C	-2.006321072	-3.7891496552	0.2557738776
H	-2.0168353118	-3.4153216722	2.3801850925
H	-1.8638383846	-3.8499113216	-1.8960015124
H	-2.4647598063	-4.7711456491	0.3391770126
C	-3.3160241806	0.439723947	-0.3979245765
H	-3.4562115605	-0.1362928731	0.5192455912
H	-4.1490272521	1.1396912493	-0.5142675078
H	-3.3013842099	-0.2454634073	-1.2481142998

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TS$_{4\text{-}5A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0021723463	-0.9242969796	0.0603246599
C	1.9282065278	-1.3850189176	0.6076418999
C	1.8179060056	-1.2754481267	-0.7715328651
C	2.266856517	-0.1436867475	-1.6890905139

C	3.48845857	0.6842852594	-1.2091190179
C	3.1337533589	1.9466050695	-0.452433723
C	2.4597149177	2.0823171985	0.69492667
C	1.9050742812	1.0496423345	1.6428901988
C	2.4640087891	-0.3897886645	1.6269731733
H	1.8755261064	-2.4006520379	0.9950511862
H	1.6693740783	-2.2226613748	-1.2899298277
H	1.439675428	0.5447649806	-1.9110338523
H	2.51735863	-0.6136754166	-2.6477898374
H	4.1587329548	0.03614216	-0.6319681017
H	4.0579818919	0.9790507222	-2.0971795584
H	3.4254505816	2.8717357806	-0.9486303769
H	2.2572364242	3.1039351651	1.018158
H	0.8080685519	1.02194082	1.5370036328
H	2.0627286213	1.4378328638	2.6583033219
H	3.5603717703	-0.3529258441	1.5578333879
H	2.2490463857	-0.8190978632	2.6123947998
S	-1.8217484963	0.1702253069	0.2151254686
C	-0.6968734451	-2.6259000264	0.2928783409
C	-0.9652513315	-3.1543750633	1.5621851822
C	-0.8931371654	-3.4329989317	-0.8355454796
C	-1.4153109268	-4.4709711039	1.6981105704
H	-0.8440647778	-2.539279969	2.4496978516
C	-1.3466239026	-4.7502037608	-0.6951660734
H	-0.7047772029	-3.0452525829	-1.8344133297
C	-1.6053725996	-5.2743950334	0.5713567744
H	-1.6252302167	-4.8647703924	2.6899885085
H	-1.4936959569	-5.3635733172	-1.581317393
H	-1.9577149487	-6.2966427048	0.6802236735
C	-2.9984970194	-0.3845279604	-1.0845120722
H	-3.1244593002	-1.4692854302	-1.038429214
H	-3.9622443006	0.0922481551	-0.888973564
H	-2.6596815449	-0.0996431272	-2.0842842503

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5A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.4957637037	0.2591913535	-0.0000277381
C	1.4351184779	0.0909519741	0.6847260147
C	1.3977771134	0.2240631014	-0.6971195829
C	1.5483484782	1.4827935041	-1.5354309668
C	3.0146194071	1.9086005597	-1.7570282195
C	3.8225677153	2.3308752341	-0.5554564836
C	3.4513016656	2.6081932509	0.7006892703
C	2.0779305351	2.5568242188	1.3372509737
C	1.6547963299	1.1355889019	1.7665278746
H	1.5457654349	-0.9279547967	1.0512527674
H	1.5288889992	-0.7006857589	-1.2596831442
H	0.9757711656	2.3167868366	-1.121345982
H	1.1057478586	1.2846868641	-2.5192722287
H	3.5466299386	1.0797390537	-2.2473666692
H	3.0260068738	2.7277804602	-2.4932261453
H	4.8866913022	2.4298578735	-0.7755623949
H	4.2525052085	2.8839153076	1.3867428794
H	1.3113605543	3.0061818797	0.700312199
H	2.0973087786	3.1734203664	2.2436793221
H	2.4334064356	0.73364383	2.4303280663
H	0.7544510423	1.2046654581	2.3966139945
S	-2.4302679446	1.1376826256	0.0565548907

C	-0.9415322106	-1.5274073066	0.1814057634
C	-1.2172918207	-2.0990049109	1.4302591314
C	-0.947001382	-2.3436001799	-0.9571566933
C	-1.4892750061	-3.4662449197	1.5362419996
H	-1.2411662334	-1.4808797943	2.3236939385
C	-1.2229928278	-3.7117309678	-0.8471026355
H	-0.7438368727	-1.9256176839	-1.940882832
C	-1.4914069684	-4.2777401113	0.3993651141
H	-1.7080962289	-3.8941788536	2.5119300009
H	-1.2239266168	-4.3319776039	-1.7406572477
H	-1.7057101933	-5.3397374598	0.4845413128
C	-3.3991529147	0.5249271151	-1.3821327488
H	-3.3959419326	-0.5681968718	-1.3970550227
H	-4.4287311199	0.8728426763	-1.2673024172
H	-3.0027603384	0.9025007736	-2.3286503612

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TS$_{5A-9A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.2450611692	-0.0778017611	0.2398296704
C	-0.9940504605	1.5141946554	-1.0305584472
C	-1.5881395997	1.9101744586	0.1629263921
C	-0.9180986359	2.6103638877	1.3275535486
C	-0.9228356079	4.1498827699	1.1611330198
C	-0.3282679913	4.7282981467	-0.1034641047
C	0.5651426219	4.2044492996	-0.9521289524
C	1.2530913302	2.8619272321	-0.8656660154
C	0.4511018295	1.6895051886	-1.4853366574
H	-1.6835181159	1.3134926402	-1.8478070108
H	-2.6734391246	2.0153049389	0.1444708935
H	0.0972656942	2.2404912203	1.4826696637
H	-1.4681237434	2.3751536919	2.2478495051
H	-1.9655398275	4.4931939709	1.2210630405
H	-0.4254559745	4.5942662331	2.0377863041
H	-0.6985938294	5.7270135892	-0.3388570007
H	0.8286451555	4.8083349128	-1.8209314051
H	1.5199582784	2.6277663488	0.1668505783
H	2.2053069433	2.9165187388	-1.4079196832
H	0.4142857079	1.8348456593	-2.5725133059
H	1.0277787146	0.7652236523	-1.3383113211
S	2.3564036475	0.2534681293	1.6024023726
C	3.2318757952	-0.5929470368	0.2814938612
C	2.3245975187	-1.0164776446	2.9228042496
C	4.3910987249	-0.0039220802	-0.241525885
C	2.7553513118	-1.7951330454	-0.2630455376
H	1.6449670844	-1.8299056722	2.661019688
H	3.3348580041	-1.3853321336	3.1150716954
H	1.9449201986	-0.5148152325	3.8172397344
C	5.0682675079	-0.6110545808	-1.3015577289
H	4.7623946658	0.9214184729	0.1890163941
C	3.4506265453	-2.4053361858	-1.3082818893
H	1.842854547	-2.2420316241	0.1227301271
C	4.6037960111	-1.8153825539	-1.832705568
H	5.9660797387	-0.1473400727	-1.7019101402
H	3.0802560557	-3.339793069	-1.7217721145
H	5.1363710576	-2.2918806762	-2.6513884252
S	-0.7673509057	-1.9119068532	1.238600366
C	-2.7505280713	-0.7553730521	-0.608574028
C	-2.2045777543	-3.0034494474	1.5730169179

C	-2.6471313159	-1.4739638512	-1.8070667214
C	-4.0207244001	-0.4785449592	-0.0875970278
H	-2.9848889065	-2.4810306655	2.131364525
H	-2.6249615149	-3.3836649639	0.6395432429
H	-1.8396524304	-3.8422656427	2.1719503314
C	-3.7988143041	-1.9047830375	-2.4732796098
H	-1.6708261938	-1.7129065648	-2.2199281042
C	-5.1705612971	-0.9141141444	-0.7565608047
H	-4.1288188548	0.0648297449	0.8482024956
C	-5.0642696357	-1.625483218	-1.952084119
H	-3.702461657	-2.4637927888	-3.4013740943
H	-6.149775821	-0.6932991368	-0.3375979146
H	-5.9575693376	-1.9634036175	-2.4705909013

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9A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.6812367528	-0.2662537412	0.3000140556
C	-0.5630858445	1.4280129681	-0.9797746197
C	-1.1584879116	1.7680207037	0.2255269336
C	-0.620679746	2.6524430482	1.3305468916
C	-0.9479754891	4.141187305	1.0747810957
C	-0.4063039258	4.7780509405	-0.183441515
C	0.561888227	4.3778004465	-1.017805114
C	1.4278150174	3.1387898738	-0.9491144113
C	0.7715014222	1.8762025273	-1.557967399
H	-1.255329383	1.0846983307	-1.7449727452
H	-2.2441311974	1.693831949	0.2437349383
H	0.4498923821	2.5233805324	1.4866505141
H	-1.1045267007	2.365810242	2.2739865102
H	-2.0417035197	4.2570244562	1.0596972718
H	-0.6133191502	4.7260602525	1.9465361711
H	-0.8997621618	5.7190312252	-0.4318900365
H	0.7490619443	5.0171167525	-1.8811795553
H	1.7533819434	2.9344456522	0.0729279529
H	2.3464967637	3.3278948704	-1.5192845973
H	0.5864648708	2.0735498565	-2.6226764731
H	1.5062212211	1.0598706217	-1.5504007764
S	1.6346570307	0.1310550665	1.1432031503
C	2.8829646073	-0.7155296713	0.1547832573
C	1.8778185149	-0.6386704418	2.7852086487
C	4.0196563197	0.0125777517	-0.22073006
C	2.7354220088	-2.0508896395	-0.2391828993
H	1.5671801255	-1.6842065162	2.7648433376
H	2.9268517891	-0.5314306059	3.0692586255
H	1.2447703424	-0.0897973686	3.4866835939
C	5.0115791691	-0.5975665736	-0.9908253609
H	4.1239787076	1.0476234664	0.0908724866
C	3.7375056134	-2.6530203258	-1.0024968062
H	1.8452006476	-2.6023418201	0.051789316
C	4.8719882314	-1.9309263548	-1.3805807045
H	5.8920413215	-0.0311891504	-1.2817965256
H	3.6256348268	-3.6902029173	-1.3066702374
H	5.6452735792	-2.4059164135	-1.9783178377
S	-0.5416721727	-2.2498402475	1.2144734075
C	-2.3708999513	-0.7390972264	-0.4000048196
C	-1.9683128279	-3.3832107398	1.0126277629
C	-2.4688739617	-1.2685519968	-1.6972095326
C	-3.5636450836	-0.516518754	0.3062063398

H	-2.8713188014	-2.9781997505	1.473801734
H	-2.171242699	-3.5898790855	-0.0401805713
H	-1.693936358	-4.3145343149	1.5172425069
C	-3.712273178	-1.5573965248	-2.2702314171
H	-1.5675053036	-1.4718481334	-2.2724576649
C	-4.8086456712	-0.8034238986	-0.2637513442
H	-3.5294498198	-0.127444016	1.3221898745
C	-4.8891033473	-1.3238968143	-1.5565456284
H	-3.7579403993	-1.9673008496	-3.2771295072
H	-5.7164939991	-0.6210189641	0.3076383438
H	-5.8556522705	-1.5479909827	-2.0004895605

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TS$_{9A\text{-}10A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.5581451206	0.8508157993	0.3550286623
S	1.220884865	1.6479036241	2.2287368017
C	-0.2749158739	2.3191076255	3.0561936513
H	-1.0239014377	1.5463210211	3.2547502839
H	0.0450004174	2.7473879805	4.0113157962
H	-0.7376147681	3.1124457391	2.462254071
S	1.3298768769	-1.3659789398	0.3454861793
C	0.57710556	-2.453896634	1.5644630356
C	3.0428061485	-1.2392767879	0.9775842373
C	0.3809379356	-2.0274859889	2.8840545325
C	0.1821054625	-3.7361600159	1.1658391763
H	3.0527916068	-0.6986624649	1.9269115753
H	3.4653502147	-2.2400046052	1.0883633607
H	3.6141160637	-0.6796420332	0.2325591617
C	-0.20757317	-2.8977394799	3.8034655913
H	0.6851324658	-1.0253275934	3.1766704311
C	-0.4153185505	-4.5949013837	2.0916934681
H	0.3467436539	-4.0564826429	0.1414950854
C	-0.6082505844	-4.1775425761	3.4100705484
H	-0.3575139543	-2.571615256	4.8291154945
H	-0.7219680125	-5.5903772808	1.7827056255
H	-1.0687755136	-4.8483990645	4.1300644502
C	-4.7308246637	-2.1552414882	-1.0139590203
C	-4.7767010803	-1.9689231379	0.3113953407
C	-3.5556885394	-2.3083057168	-1.9491474749
H	-5.6926873145	-2.2103316937	-1.52672353
C	-3.638211221	-1.8445285676	1.3021222354
H	-5.7709378515	-1.8677397811	0.7479360902
C	-2.1545693039	-1.9330640927	-1.4181410165
H	-3.7618520792	-1.701416126	-2.8432990091
H	-3.5261733197	-3.348280059	-2.3131229983
C	-3.0148763953	-0.4325844449	1.3671670512
H	-2.8593550471	-2.5880765557	1.1185313364
H	-4.0267344961	-2.0725660616	2.3026035617
C	-2.0319579267	-0.4754985151	-1.0315235012
H	-1.8798093252	-2.5939572139	-0.5936719954
H	-1.4332982275	-2.1415788267	-2.2187728433
C	-2.3961028562	0.1314747843	0.110669589
H	-3.7921935942	0.2756184561	1.6890369152
H	-2.2638353362	-0.4196661645	2.172330557
H	-1.668351775	0.1789440029	-1.822397713
H	-2.2648397442	1.21274413	0.1389334692
C	0.2681070732	2.41652167	-0.5516070172
C	0.3017669174	2.0505182012	-1.9103888311

C	0.0620749717	3.7659501956	-0.2427663355
C	0.0840804647	2.9863455721	-2.9269512477
H	0.4998121041	1.0149481361	-2.2022788278
C	-0.1605536072	4.7062278686	-1.2539686107
H	0.0883033067	4.1003819306	0.7897767553
C	-0.1545538567	4.3212718666	-2.5968008619
H	0.1100645005	2.6749494136	-3.9689649121
H	-0.328331926	5.7483806667	-0.9903497916
H	-0.3221554978	5.0571893785	-3.3790909135

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10A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.8047498998	-1.3271294446	0.0618215474
S	0.4949679442	-2.5133770221	-1.0725354941
C	-0.0154706604	0.3404147651	0.1313543387
C	0.2530340541	1.0853976439	-1.027259514
C	0.3424430739	0.8871984039	1.373896735
C	0.8349906072	2.3536756343	-0.9415527803
H	0.0209779507	0.6744490181	-2.0054628783
C	0.9337553303	2.1521183465	1.4580122171
H	0.1593351565	0.3334461468	2.2925432657
C	1.178205756	2.8921611495	0.3003452993
H	1.0324618062	2.9156807896	-1.8519026353
H	1.1992355249	2.557912489	2.4319278924
H	1.6363028012	3.8758968139	0.3644216857
C	1.9539831087	-2.9042218393	-0.0178778978
H	2.6300504655	-3.5372084716	-0.5987943665
H	2.4781261055	-1.9819928793	0.2467781955
H	1.6735858886	-3.4345388949	0.8958831174
S	-2.616773546	-0.7640353234	1.2413915468
C	-3.6942602004	0.2688793245	0.2350801252
C	-3.6113318021	-2.3078135794	1.310047125
C	-3.5544984502	0.306001737	-1.1561258918
C	-4.6643786124	1.0506250622	0.8712465951
H	-4.5608348612	-2.1031867105	1.8096486229
H	-3.7906085293	-2.7017604802	0.3071772776
H	-3.0407354601	-3.0345671534	1.894255396
C	-4.4033843472	1.1140557033	-1.9126184753
H	-2.7798369261	-0.2862914476	-1.6322794731
C	-5.5114954666	1.8547851406	0.1072266257
H	-4.7502951826	1.032903839	1.9537749941
C	-5.3825501476	1.8857811694	-1.2830350925
H	-4.2944639275	1.1440047677	-2.992979411
H	-6.2657671077	2.4621859594	0.5994999106
H	-6.0399724464	2.5165513427	-1.8748086032

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5C B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.8611240748	-0.0894362658	1.0417557991
S	0.735014059	0.2394345731	2.3900980181
C	0.4641478941	1.7133249168	3.4522754763
H	-0.3941055408	1.5819234431	4.1165564334
H	1.3627037896	1.8535098548	4.0585250169
H	0.3129171195	2.600186905	2.8323265453
C	-5.2158303075	-1.3060045954	-1.14795709
C	-4.4661722514	-0.92029668	-2.1884790667
C	-5.1303777339	-0.955291797	0.3168383568

H	-6.0414069699	-1.9831011678	-1.3734918035
C	-3.2535392831	-0.0133848686	-2.2294422785
H	-4.7427789911	-1.341041732	-3.155824097
C	-3.8689263812	-0.2192695088	0.8108261349
H	-5.2446761658	-1.8853973718	0.8939717392
H	-6.0092457029	-0.3476441637	0.5849638906
C	-1.9378032871	-0.7255419651	-1.8513809279
H	-3.3810847628	0.8827080787	-1.6182095215
H	-3.1353594305	0.3504715225	-3.2572540812
C	-2.6070413594	-1.0449154622	0.6800749477
H	-3.7687746449	0.7417010016	0.3063901454
H	-4.0131850978	0.011877866	1.8742335168
C	-1.7917545848	-1.229590522	-0.42930662
H	-1.8249334048	-1.6045487087	-2.5019787906
H	-1.0979701034	-0.0638265794	-2.0973815568
H	-2.5119239994	-1.8070451746	1.4628248533
H	-1.1185275974	-2.090174108	-0.3647429151
C	-0.8041831686	1.5905184922	0.2675375437
C	0.0929662384	1.8905470301	-0.7674784517
C	-1.7209282288	2.5712151429	0.6712797897
C	0.0457125933	3.1314880325	-1.4105131883
H	0.8475821695	1.167092407	-1.0639514816
C	-1.7657719777	3.8128607873	0.0253674369
H	-2.4036266975	2.3847922533	1.4969540503
C	-0.887436177	4.0948535828	-1.021348398
H	0.7500384001	3.3464200998	-2.2109164101
H	-2.4891523552	4.5584831478	0.3476496524
H	-0.9200279839	5.0599225335	-1.5198486682

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TS$_{5C\text{-}10B}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0506365701	-0.1623828318	0.6276363983
S	-0.0751948685	0.2323288869	2.7078482036
C	1.4027319533	1.1731254255	3.2625270812
H	1.389168329	2.1820271626	2.8396314293
H	1.3488453449	1.2541855726	4.3521748692
H	2.3416591424	0.680297832	2.9945950102
S	1.5127089096	-1.58995986	-0.7900199734
C	3.1613819223	-0.8965716041	-0.6002470566
C	1.6049196315	-3.0182638866	0.3619709089
C	4.2567124732	-1.506645439	-1.2235065144
C	3.33027651	0.2827575909	0.1302838327
H	2.4173587272	-3.6825673948	0.0602239716
H	1.7532206603	-2.6766312606	1.3894084261
H	0.6561369536	-3.5565693115	0.2874491572
C	5.5264601923	-0.9441922719	-1.0885537717
H	4.1150166581	-2.4092452322	-1.8112994089
C	4.601253253	0.8472328918	0.2500417495
H	2.4581289529	0.7408447394	0.5848889465
C	5.6995802807	0.232075468	-0.3535017138
H	6.3790068382	-1.4183511732	-1.5670833468
H	4.7297907417	1.7659020984	0.8154224546
H	6.6889908156	0.6707988307	-0.2581099616
C	-5.2445722281	-1.3381495311	-0.2779761563
C	-4.880847103	-0.9036955356	-1.4915343918
C	-4.6073206588	-1.1343922347	1.0752330994
H	-6.1557399519	-1.9376221798	-0.233534392
C	-3.6826407126	-0.0677266625	-1.8894697847

H	-5.5183779028	-1.2087155484	-2.3222304909
C	-3.1739209646	-0.565286617	1.1295738861
H	-4.6211087706	-2.1020079202	1.5995828164
H	-5.2598602483	-0.4804364453	1.6758598132
C	-2.3769992295	-0.8788727514	-2.0411063137
H	-3.520249639	0.766432955	-1.2038201649
H	-3.889632072	0.3922987716	-2.8636036149
C	-2.1550298404	-1.4779653285	0.4806835896
H	-3.1470917851	0.4348144268	0.6971203633
H	-2.902313597	-0.4387306983	2.1830839596
C	-1.875263537	-1.633531954	-0.8339691466
H	-2.512530667	-1.6151734567	-2.8461295067
H	-1.5863663676	-0.1992676772	-2.3938831397
H	-1.7365194297	-2.2310677344	1.1529248061
H	-1.2102839569	-2.4590127804	-1.0918227553
C	-0.3034719845	1.5009923187	-0.1165608833
C	0.316464274	1.746941078	-1.3561474071
C	-1.1629537562	2.4936968766	0.3901989357
C	0.0753500915	2.9266016239	-2.0696881829
H	1.0074680545	1.0243970454	-1.7849714353
C	-1.4044714916	3.6718099766	-0.3237354355
H	-1.6396635704	2.3526010109	1.3542595382
C	-0.7890757022	3.894008638	-1.5571520353
H	0.56867079	3.0849985568	-3.0263094816
H	-2.0748667734	4.4209049287	0.0924413503
H	-0.976154121	4.8117466151	-2.108909131

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10B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	1.3955145635	1.1455149194	0.9448501744
S	1.0690927223	1.4213779339	2.9940883918
C	1.5606337843	3.1470646567	3.412282565
H	0.92088951	3.854471136	2.8780410025
H	1.4176117498	3.2874468905	4.4869957601
H	2.6060519819	3.3500019691	3.1653697087
S	2.3221887716	0.4469298679	-0.960482387
C	3.6626994049	-0.6655964082	-0.4937975925
C	1.1478934881	-0.7174122254	-1.7540347601
C	4.5070675641	-1.1831234998	-1.4831872641
C	3.8864797965	-0.9646356533	0.8536914805
H	1.5743605351	-1.0804426079	-2.6911852227
H	0.9235879427	-1.5522385674	-1.0873282641
H	0.2389266133	-0.1450270626	-1.9497788999
C	5.5598354597	-2.023321199	-1.1206654915
H	4.3450332394	-0.9267961408	-2.526396441
C	4.9506703761	-1.7951444337	1.2092261056
H	3.2388491185	-0.5455246713	1.6208874876
C	5.7832399548	-2.329281273	0.2246030975
H	6.2123472344	-2.4297331551	-1.8884059767
H	5.1231667711	-2.0247409602	2.2568034905
H	6.6087562242	-2.9780015135	0.5036536964
C	-0.0414631667	1.9420144596	0.095770829
C	0.1605497164	3.0556115518	-0.735947649
C	-1.3493052795	1.4557244303	0.2521951904
C	-0.9116940334	3.6568002767	-1.4041833075
H	1.1593375826	3.4649727983	-0.8735098084
C	-2.4189866162	2.0517360446	-0.4236312487
H	-1.5442035784	0.6173906177	0.9153497817

C	-2.2051501618	3.1544779367	-1.253558703
H	-0.7313609489	4.5175404095	-2.0446313403
H	-3.4245595631	1.6592581447	-0.2882139749
H	-3.0387517573	3.6204383278	-1.7727634304

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TS_{5A-11} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.5725228469	0.6124787783	-0.0936931529
S	-1.230232856	2.4583759236	-0.8005510962
C	-2.0873579291	-0.4163763322	-0.038013016
C	-2.0982113494	3.2803791644	0.5993499219
C	-2.3841213002	-1.0477394745	1.1818542444
C	-2.9103655964	-0.6718872214	-1.1452006291
H	-2.9752852952	2.6981133161	0.8926891875
H	-1.4486027789	3.4225916274	1.4670412088
H	-2.4314113743	4.2599650593	0.2451105982
C	-3.4608319983	-1.9340241832	1.2857973762
H	-1.7781172709	-0.8563910262	2.0665733941
C	-3.9840433413	-1.5609550442	-1.0404769243
H	-2.7212056828	-0.1702701339	-2.0892070867
C	-4.2621786264	-2.19464058	0.1728977061
H	-3.6724573467	-2.4175198099	2.2369704256
H	-4.6100997696	-1.7515630307	-1.9092629646
H	-5.1021156484	-2.8800189335	0.2524934824
C	2.0999234576	-1.9827920042	-0.1048760007
C	3.1050226615	-1.8443411059	-0.9784673684
C	1.3419677478	-0.944420461	0.6819809516
H	1.7469449731	-2.9972673116	0.0793345322
C	3.8122712903	-0.5880275701	-1.4360503401
H	3.4980178062	-2.7683726178	-1.4026657385
C	1.9594007824	0.46881834	0.8038056869
H	1.1688054657	-1.3353778558	1.6932455751
H	0.3079315254	-0.9468330508	0.2421399725
C	4.91874195	-0.1169932431	-0.4660011233
H	3.108099982	0.2255936697	-1.6263046219
H	4.2888128159	-0.7929843246	-2.4021588022
C	3.3150268296	0.472510493	1.4788223823
H	2.0018070032	0.9508014959	-0.1774458117
H	1.2819307249	1.0863677461	1.4093662181
C	4.5189043102	0.2347071409	0.9452867948
H	5.6850632827	-0.9034291119	-0.404582876
H	5.4337157748	0.7477463709	-0.9134266488
H	3.2868464881	0.6906471415	2.5458075414
H	5.3668381397	0.3006441591	1.6284940014

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11 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	1.0597850427	-0.8501320319	-0.0197543255
S	2.2433628744	-2.4253268168	-0.5945756448
C	1.9030721368	0.7386655143	0.0943917673
C	3.1518229329	-2.9556162973	0.9181403419
C	1.9062327088	1.3425201292	1.3635332291
C	2.3484214127	1.4739171388	-1.0151725605
H	3.8288488477	-2.1650774501	1.2513337929
H	2.4793724706	-3.2305852851	1.7338353273
H	3.7474385039	-3.8303822742	0.6420355762
C	2.3009765121	2.6764312428	1.5108598537

H	1.6094635632	0.7804851166	2.2471736969
C	2.7518894233	2.8021842147	-0.8624031047
H	2.3882625371	1.0092585791	-1.9964891702
C	2.7246237734	3.4055740083	0.3985730998
H	2.2901094047	3.1387267755	2.4951436475
H	3.0920090142	3.3665086513	-1.7274984615
H	3.0436998415	4.4381237847	0.5144429347

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$TS_{11\text{-}10A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.8607410288	0.3810671341	-0.9598481551
S	0.8774263564	2.4239864783	-1.2513440569
C	2.4647093589	-0.2379067969	-0.4062634165
C	0.6431532091	3.1754189052	0.4154409747
C	3.6875332488	-0.0286249008	-1.0592150699
C	2.3933802937	-1.1555473486	0.6547294299
H	0.5639021698	4.2567093424	0.2705048973
H	-0.2632814546	2.8168096677	0.9090837046
H	1.5095849578	2.9710332265	1.0488104429
C	4.8161178973	-0.7597480193	-0.6797309052
H	3.7612266758	0.7048553721	-1.8564392596
C	3.5255314962	-1.8913863682	1.0233206647
H	1.4650837982	-1.3055114837	1.2037634838
C	4.7361362975	-1.693514944	0.3575349992
H	5.7608730197	-0.5970974062	-1.1932039368
H	3.4610489115	-2.6069398692	1.8397309424
H	5.6180261099	-2.2563296056	0.6525064402
S	-1.3970536303	-2.3304207477	0.5810282238
C	-2.736937828	-1.1412955437	0.4646714768
C	-0.7409535824	-2.3006928231	-1.1247313881
C	-2.5057796572	0.168394496	0.0257005551
C	-4.0217702762	-1.5176151637	0.874229103
H	-1.5003561311	-2.5910762007	-1.8545002748
H	-0.3631143315	-1.3012147692	-1.3987291546
H	0.0970953392	-3.0010279211	-1.1591755967
C	-3.5530784421	1.0861267064	-0.0278328771
H	-1.5043572412	0.4694522569	-0.2760732325
C	-5.0631088449	-0.5869440035	0.8438858648
H	-4.2029172137	-2.5348455301	1.208379062
C	-4.8341824517	0.7119937013	0.3871261422
H	-3.3629439408	2.0952615537	-0.3828458042
H	-6.0576244476	-0.8845338536	1.1652521323
H	-5.6486276953	1.4302584582	0.3542155881

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$TS_{5A\text{-}9B}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.7686387912	0.9266101377	0.0874691464
S	-2.1254045157	2.4720099515	-0.3855441167
C	-1.502776292	4.1960070752	-0.4171308715
H	-1.0658316769	4.4825520629	0.5416211167
H	-0.7677976627	4.3514239099	-1.2092561083
H	-2.3783221699	4.8235556487	-0.6136246286
S	1.753949361	-1.4743123467	1.7620015584
C	2.6461716183	-1.8583545919	0.2600780337
C	1.3083750053	-3.1155757562	2.4205298541
C	3.2716236756	-0.7801101698	-0.3880225381
C	2.7365125016	-3.1419195519	-0.2940416038

H	0.5996085841	-3.6397889691	1.7732570426
H	2.1973013195	-3.7320695194	2.5795783532
H	0.8313371976	-2.928768178	3.386200463
C	3.9720467897	-0.9912200829	-1.5733598265
H	3.2123554846	0.218118163	0.0353097751
C	3.4489727091	-3.3412867083	-1.4801178085
H	2.2602240319	-3.990428868	0.184959917
C	4.0672172322	-2.2716590892	-2.1259949042
H	4.4484319255	-0.1465743358	-2.0637640358
H	3.5142347052	-4.3429447416	-1.8973444123
H	4.6182940031	-2.4322088741	-3.0482808323
C	-1.4461420279	-0.9211607926	-0.5531205445
C	-1.9071262503	-0.7177157461	0.7331171357
C	-2.189562778	-0.9507481311	-1.8765998676
H	-0.4493100901	-1.371921325	-0.6160621993
C	-3.3152407665	-0.4243582778	1.2091198156
H	-1.2372138531	-1.0630110805	1.5248550876
C	-3.7317501309	-0.9528895601	-1.8255446779
H	-1.8598349097	-1.8604784704	-2.3985766476
H	-1.8569146391	-0.1124986395	-2.5027938405
C	-4.1733536619	-1.697044611	1.3569931683
H	-3.8166909639	0.3028137094	0.5706173901
H	-3.2477743918	0.0535423613	2.1939916708
C	-4.314369365	-2.1948823021	-1.1836733991
H	-4.0888837128	-0.0349704709	-1.3537110829
H	-4.0866882476	-0.9053552229	-2.8622870862
C	-4.4808813081	-2.492197011	0.1116850039
H	-3.6833692404	-2.3733493326	2.0744785651
H	-5.1240467436	-1.4173979946	1.838463964
H	-4.6143233471	-2.9676227182	-1.892585383
H	-4.9206720941	-3.4674252881	0.3285484264
C	0.6741689195	2.0834659475	0.1792829554
C	1.406828808	2.4690117032	-0.9567426523
C	1.2443387114	2.3144167357	1.4437322336
C	2.6798400551	3.0346130745	-0.8357638468
H	0.9809460856	2.3337882902	-1.9485271476
C	2.5179399059	2.8809033837	1.5683149521
H	0.6948527242	2.059950858	2.3479526085
C	3.2405467887	3.239700272	0.4281575531
H	3.2314118733	3.3215036846	-1.7286377874
H	2.9418949577	3.0456804242	2.5563207139
H	4.2265546567	3.6873783645	0.5237793449

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9B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.4684560815	0.4219779551	-0.1636639877
S	-1.4827313228	2.0122267175	0.9224722647
C	-0.6393200164	3.6386910948	0.9644981005
H	0.2709024563	3.6112066705	1.5666107107
H	-0.3906939235	3.9945854009	-0.0381456877
H	-1.3525197306	4.3331749038	1.4204269568
S	0.9038829341	-1.0753448406	-1.3741095117
C	2.3455840685	-1.58452162	-0.4238632549
C	0.2499167261	-2.7382638742	-1.8018270273
C	3.6140281479	-1.2631278282	-0.9134080001
C	2.2104107437	-2.2850303666	0.7799923892
H	1.0029969586	-3.261898121	-2.3947821063
H	0.0107308126	-3.3256567628	-0.9124577613

H	-0.6517430126	-2.6072769119	-2.4044700625
C	4.7492466676	-1.651465877	-0.1989433731
H	3.7081386929	-0.7008595489	-1.8364269766
C	3.3488761771	-2.6802013305	1.4820427443
H	1.2236890469	-2.5133437538	1.1728407208
C	4.6192644612	-2.36361585	0.9938802983
H	5.734727071	-1.3952988533	-0.5775846213
H	3.2425507895	-3.2252476312	2.4159659993
H	5.5043228854	-2.6668267807	1.5462620449
C	-2.3257469419	-0.4165771135	-1.0149420888
C	-2.0701166967	-1.0353555528	0.1842707233
C	-3.4369258005	0.5374915011	-1.4138170988
H	-1.8447009109	-0.8583830271	-1.8873554609
C	-2.8313838133	-0.9188415086	1.4864543765
H	-1.4469116046	-1.9283441423	0.1389033269
C	-4.6587219666	0.6416960428	-0.4762905932
H	-3.7866509894	0.1977191452	-2.3997250808
H	-3.024384947	1.541682797	-1.5621648498
C	-4.0382909049	-1.8798699547	1.5403371822
H	-3.1415160947	0.1053545019	1.6845330275
H	-2.1533875428	-1.1835183617	2.3074266163
C	-5.4051660909	-0.6628872999	-0.2938741803
H	-4.3504955274	1.0815494927	0.4734556354
H	-5.3442739099	1.3691519289	-0.9285845739
C	-5.1414839274	-1.6877219446	0.5274371632
H	-3.6729904506	-2.9142708227	1.4440380465
H	-4.4717299839	-1.8283310617	2.5518528146
H	-6.2706161813	-0.7851692618	-0.9465985775
H	-5.8293491	-2.5339863715	0.4807716782
C	1.1561669346	1.4086729533	-0.0224801311
C	1.6803987862	2.0882139027	-1.1369344425
C	1.9210244577	1.4230728219	1.1577345683
C	2.9139157064	2.7481195231	-1.0796257917
H	1.1222440798	2.1137903387	-2.0715299882
C	3.1562989954	2.0731662475	1.2199760318
H	1.543508236	0.9290490946	2.0501481821
C	3.6594281706	2.7403936252	0.0997798726
H	3.2887440212	3.2692862275	-1.9584756685
H	3.7244577505	2.0647807767	2.1480267205
H	4.6173066944	3.2526507102	0.1487667011

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TS$_{9B-10A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.1818800154	0.2014058187	0.2557239317
S	-0.8324159169	1.1853166531	1.8435126947
C	-1.2480206349	2.9178440457	1.391331859
H	-0.3354138093	3.4724906921	1.1600604675
H	-1.9294055257	2.9738302085	0.5375667779
H	-1.7325992525	3.3774572524	2.2573853244
S	1.2770180072	-1.2483018023	-1.0898429924
C	2.7889814108	-1.6912000469	-0.213901519
C	0.5257000062	-2.9210941103	-1.1928853128
C	3.9096449864	-2.0713077105	-0.9586639954
C	2.8425514412	-1.6677053638	1.1832864848
H	1.2332322462	-3.5826150557	-1.6974780088
H	0.2920983248	-3.3117996244	-0.2003759468
H	-0.3860670197	-2.8442275682	-1.7875201206
C	5.0813684021	-2.4478414773	-0.2996412387

H	3.8657982871	-2.0658441377	-2.0438407951
C	4.0162579465	-2.0461758276	1.8351056695
H	1.9755004812	-1.3380345756	1.7471160083
C	5.1345164723	-2.4382140281	1.0955858585
H	5.9533501993	-2.7411710473	-0.877504526
H	4.0577079025	-2.0270255686	2.9204985395
H	6.0486228801	-2.7283771599	1.6060780445
C	-2.4948370663	-0.8363356801	-1.0940787046
C	-2.6654037399	-1.7174652457	-0.0941528501
C	-3.0207685324	0.5671046046	-1.275311647
H	-1.9267742875	-1.1878932326	-1.9583926314
C	-3.4322187132	-1.5565921087	1.1980505763
H	-2.2274967514	-2.7053049318	-0.2429966332
C	-4.1512225304	1.0369633201	-0.3366075315
H	-3.3633289821	0.6550314206	-2.3169886174
H	-2.1751770485	1.2655122908	-1.1837282007
C	-4.9488288006	-1.8158368857	1.0583226228
H	-3.2389104306	-0.5780469314	1.6415134362
H	-3.0441666027	-2.2868412987	1.919863376
C	-5.4250109385	0.2287754281	-0.4569258325
H	-3.779887321	1.0636325504	0.6896212159
H	-4.3789072855	2.07793611	-0.598871838
C	-5.7399817796	-0.9381553963	0.1189303398
H	-5.0973002561	-2.8583964661	0.7385361049
H	-5.4023403658	-1.760891706	2.061052687
H	-6.1763447853	0.6569647927	-1.1215971845
H	-6.727820466	-1.3409016072	-0.1120951207
C	1.5007717666	1.4827833761	0.0261023442
C	1.5873229549	2.0947141194	-1.2359194422
C	2.4084623243	1.882110636	1.0194558561
C	2.5606858517	3.0636420009	-1.5025584822
H	0.8962096824	1.819285353	-2.0303752438
C	3.3857764414	2.844791533	0.7505622066
H	2.3484313838	1.4490138891	2.0128953918
C	3.4663867647	3.4403772395	-0.510323075
H	2.6089668612	3.5204718445	-2.4887980484
H	4.0805153537	3.1366095697	1.5353388113
H	4.2236894482	4.1929928457	-0.7149220901

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TS10A-12A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	1.0770961506	-0.2155028389	0.3202220919
S	1.8912705292	1.1191894745	1.7424789863
C	2.5827013996	-1.2480088717	0.034133169
C	3.193827989	-1.20752606	-1.2309726026
C	3.1161462936	-2.1151440998	1.0003699614
C	4.2871773437	-2.0292186821	-1.5295718762
H	2.8200603259	-0.5353138398	-2.0018128767
C	4.2047299149	-2.9399744306	0.7002055112
H	2.6928368959	-2.140714231	2.0006641939
C	4.7935389459	-2.9031773874	-0.5659780213
H	4.7412611531	-1.9830578775	-2.5172584401
H	4.6009006215	-3.6050432182	1.4647074213
H	5.6432234195	-3.5411077104	-0.795583105
C	2.9849282043	2.2828327743	0.8267021092
H	2.4456985094	2.8455711461	0.0590801204
H	3.4056513789	2.9873947383	1.5495939367
H	3.8042059718	1.7319442609	0.3568461097

H	-0.6169080514	1.3636388691	-0.457399001
Si	-1.4533417709	2.6118762123	-0.3957910087
C	-1.9071929308	2.920039506	1.4106228243
H	-2.399171423	3.8921591391	1.5386065967
H	-2.5901836986	2.1487752192	1.7853464693
C	-0.4170379095	4.0340784547	-1.0894962962
H	0.4803529132	4.2005189486	-0.4828326612
H	-0.9894490079	4.9700795163	-1.1000804367
C	-2.9951390453	2.332153018	-1.4585116888
H	-3.6537694452	3.209499517	-1.4389833756
H	-2.7276124304	2.1420541644	-2.5048042804
H	-1.0067827802	2.9059257336	2.0353234724
H	-0.0946324434	3.8305808033	-2.1174975101
H	-3.5734551561	1.4726718685	-1.1000504092
S	-0.2817667065	-1.4837215364	-0.9787224455
C	-1.8910520014	-1.5167461286	-0.1691384854
C	0.1858149078	-3.2521702357	-0.849562877
C	-2.9985702871	-2.0218815552	-0.8602942191
C	-2.0398351818	-1.0158969216	1.1286232718
H	0.2274869986	-3.5646030231	0.1951809872
H	-0.5398502862	-3.8501444258	-1.404573202
H	1.1766353967	-3.3451007256	-1.2966869922
C	-4.247952812	-2.0496809394	-0.2391024889
H	-2.8834875411	-2.3866637662	-1.8769914285
C	-3.2944430236	-1.0383804605	1.7406325813
H	-1.179603553	-0.6032744263	1.6482645645
C	-4.3972920179	-1.5588464938	1.0606462977
H	-5.1060162743	-2.4463930036	-0.7745444048
H	-3.4055475295	-0.6513107275	2.7495531189
H	-5.3721254861	-1.5779784375	1.539683768

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12A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.5521838478	0.5182110904	0.0679941311
S	1.604293988	1.9005832145	1.3557701512
C	1.9880044534	-0.6728047743	-0.0283928434
C	2.9149253449	-0.6059018528	-1.0843943937
C	2.1340433857	-1.7245375771	0.8934170058
C	3.9305525712	-1.5584367661	-1.2254798047
H	2.857091546	0.2052501577	-1.8084569155
C	3.1487222096	-2.6786905473	0.7575297552
H	1.4560530725	-1.8018052265	1.7414877654
C	4.0502900673	-2.6026449925	-0.3063403905
H	4.632495313	-1.4793352449	-2.0533925962
H	3.237010693	-3.4798190538	1.4888177588
H	4.8407357172	-3.3414334152	-0.412042365
C	3.3863134183	1.5497326684	1.6053936593
H	3.9371797953	1.5594680309	0.6619639448
H	3.7715346	2.3442126583	2.2518234839
H	3.5396882539	0.5843898246	2.0928878818
H	-0.8713598111	1.4971736541	0.2994333889
Si	-1.2853646495	2.8079612708	-0.3921487158
C	-1.2993841987	4.0863384718	0.983632642
H	-1.5461251837	5.0802262686	0.5898749082
H	-2.0363611559	3.836410951	1.7551556244
C	-0.1427357246	3.2776992098	-1.8120259667
H	0.8723047286	3.4635674241	-1.4494072909
H	-0.5150167674	4.1945936328	-2.2888245024

C	-3.0136530602	2.4078172372	-1.0395907087
H	-3.4574655584	3.2888923212	-1.5201895366
H	-2.9803178434	1.6035921094	-1.7831431872
H	-0.3124010152	4.1336036605	1.4545833017
H	-0.1034176634	2.497950508	-2.5808004934
H	-3.6858401164	2.0938713272	-0.2331696069
S	-0.8207952267	-0.7502064609	-1.2248413586
C	-2.1509947578	-1.3964580424	-0.1947924182
C	-0.0589265244	-2.3093659288	-1.8050841405
C	-3.3248553175	-1.8505936134	-0.8086810156
C	-2.0308798695	-1.4199879629	1.1989947588
H	0.3266715324	-2.8809998135	-0.9601890209
H	-0.8076946323	-2.876149422	-2.3621516272
H	0.7718980114	-2.0346652566	-2.4570717727
C	-4.3678296364	-2.3480391758	-0.0268209563
H	-3.4206017227	-1.8103503298	-1.8900748305
C	-3.0829465238	-1.9101574079	1.9750462563
H	-1.1225061511	-1.0556317603	1.6687753262
C	-4.2485012019	-2.3772030485	1.3649162359
H	-5.2766618434	-2.7033050786	-0.5046288863
H	-2.9878420057	-1.9272032691	3.057113934
H	-5.0645673885	-2.7592336702	1.9719164309

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TS$_{12A-13A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.4781170189	0.0331363517	-0.3222826953
S	-1.754332262	1.4458782594	-1.3508358522
C	-1.8042532131	-1.3199877219	-0.0504998621
C	-2.2982196208	-1.6413195012	1.2287893232
C	-2.3448116427	-2.0451727555	-1.1314208187
C	-3.2749534586	-2.6257698816	1.4226927191
H	-1.9183687337	-1.1161713686	2.1051066668
C	-3.3148422025	-3.036264295	-0.949531824
H	-2.0073936813	-1.8307598953	-2.1449962062
C	-3.7869081628	-3.3304061735	0.3323061061
H	-3.6337403489	-2.8424888304	2.4271441631
H	-3.7073077755	-3.5755964059	-1.8097085607
H	-4.5438697904	-4.0972515634	0.4779481493
C	-3.5197152009	1.3062152855	-0.8688004773
H	-3.6359383281	1.3174717887	0.2155965237
H	-4.0581839855	2.1498460194	-1.3077167301
H	-3.9122184453	0.3644725656	-1.255446457
H	0.5494468915	1.1646693167	-0.571326509
Si	-0.3943284992	2.5402308601	0.2930798896
C	0.660343083	3.7430171677	-0.7235075474
H	0.6530968988	4.7324649916	-0.2484584065
H	1.6979627913	3.3992424463	-0.7869523162
C	-1.8590568424	3.5293494252	1.033799171
H	-2.4558931819	4.0338961187	0.2656264476
H	-1.4671890929	4.2959711933	1.7163111289
C	0.5323960551	2.0602238295	1.9009188175
H	0.6442698228	2.9623055846	2.5184760736
H	-0.0203171217	1.3295202765	2.5032995615
H	0.2771562283	3.8600234777	-1.742424304
H	-2.535457038	2.8974204012	1.6227999131
H	1.5291996352	1.6538941768	1.7016935303
S	1.055896796	-1.2433985051	0.6374875457
C	2.7493100179	-0.7841502129	0.2145682938

C	1.0180447204	-2.9275450343	-0.0846490159
C	3.740570329	-0.9693372276	1.1848501884
C	3.0816028149	-0.267142748	-1.0423924012
H	1.1920438318	-2.889526405	-1.1619790074
H	1.7869879411	-3.5302920754	0.4033065439
H	0.0260270899	-3.333572043	0.1141858482
C	5.0672296455	-0.6451867582	0.8923654272
H	3.4728306599	-1.3600220561	2.1622907283
C	4.4095216688	0.0516391689	-1.3284979509
H	2.3038309435	-0.1012097715	-1.7807880013
C	5.4024575386	-0.1370121039	-0.3635981585
H	5.8349303037	-0.7860674443	1.64812461
H	4.6666733918	0.4534416744	-2.3046345741
H	6.4343845485	0.1173253979	-0.5892786939

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13A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.9910075077	-0.0596093771	-0.2960727691
S	-1.8656997202	-1.9559434485	0.30536721
C	0.1199317807	1.8219197639	-0.6402242193
C	0.6433782312	2.2675353507	0.5807612607
C	0.7884118354	2.1230042304	-1.8352677162
C	1.8639058565	2.9441678353	0.6105988705
H	0.1003414742	2.0889433765	1.5033995567
C	1.9985690134	2.8144342728	-1.8041449861
H	0.3625304826	1.812962473	-2.7848669951
C	2.539606251	3.2195843853	-0.5799934297
H	2.2795918206	3.2684212008	1.5603825498
H	2.5153547333	3.0448531333	-2.7318029039
H	3.4809400553	3.7623096377	-0.5563500922
C	-2.6872733007	-2.5733115455	-1.22015833
H	-3.0516368175	-3.5835244481	-1.0104609732
H	-3.5422786669	-1.9468688246	-1.4875377729
H	-2.0059468828	-2.621027137	-2.0753269939
H	-0.971072799	1.5462025844	-0.7103659221
Si	-2.8475205101	0.7369554391	0.7460531378
C	-2.9378305531	2.6500963942	0.5312038413
H	-3.0571323692	2.9424295428	-0.5199410251
H	-3.8168533467	3.0238672196	1.0745782216
C	-4.5490763071	0.1738532522	0.0996122116
H	-4.7505341439	-0.8775199414	0.323113916
H	-5.3331110903	0.781049242	0.571963048
C	-2.7516274921	0.474437706	2.6317300438
H	-3.6073218825	0.9602442625	3.1203700898
H	-2.7634875245	-0.5875496884	2.8941862959
H	-2.0626471689	3.1807855875	0.92197633
H	-1.8409427197	0.918637425	3.0535344781
H	-4.638336488	0.3195402828	-0.9842623021
S	1.0516630907	-1.1056985896	-1.4519935581
C	2.2282322616	-1.1136140274	-0.090714208
C	0.8399502596	-2.9017307747	-1.7148741173
C	1.921986356	-1.7364031735	1.1269705028
C	3.4605623081	-0.4746045928	-0.2629999643
H	1.8213926806	-3.3789188347	-1.7503036324
H	0.220428506	-3.3272718042	-0.9208097986
H	0.3410817944	-3.0273437825	-2.6793866918
C	2.8596255726	-1.7267671654	2.1606513315
H	0.9596188884	-2.2215322135	1.2613467627

C	4.3863868842	-0.457471781	0.7823526646
H	3.6887849492	0.0054733736	-1.2091073471
C	4.0900326831	-1.0863234943	1.9927207775
H	2.6227356678	-2.2148434925	3.1022463741
H	5.3429541297	0.039678805	0.6448556886
H	4.8148957247	-1.0788876394	2.8022795849

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14 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0690153614	0.3703093992	0.0843531533
C	0.6124493667	2.1252122588	0.037360301
C	1.4484277424	2.6135088062	1.063997956
C	0.5932116889	2.8636510223	-1.165098092
C	2.2520715805	3.7440537229	0.8893045782
H	1.4784300682	2.1014995925	2.0262015581
C	1.3934532241	3.994134211	-1.3536267456
H	-0.0601049128	2.5528849099	-1.9817525719
C	2.2268597934	4.4369249055	-0.3234845082
H	2.8932630997	4.0887423556	1.6981680351
H	1.3645178731	4.5333293445	-2.2984776341
H	2.844958167	5.3208653634	-0.4616510663
H	-0.3141899946	-1.1367251223	-0.008414085
S	-1.9057495133	0.687985354	1.0175081105
C	-3.2417521082	-0.2727957777	0.2679582522
C	-2.5656490385	2.3749858279	0.7161454908
C	-4.4791253001	-0.3096563807	0.921089747
C	-3.0466073557	-0.9785562453	-0.9202621488
H	-2.6635725361	2.5692836093	-0.3531899804
H	-3.5357632331	2.4660456353	1.2102007198
H	-1.8473878139	3.0720494379	1.1492050082
C	-5.5309432905	-1.0377952912	0.3638711147
H	-4.6194554933	0.2180162371	1.8605503063
C	-4.1024439655	-1.7089900062	-1.4678328981
H	-2.063456899	-0.9714030917	-1.3764130794
C	-5.3447419264	-1.7362569712	-0.8315342487
H	-6.491507926	-1.0676597508	0.8707424534
H	-3.9498289819	-2.2594148342	-2.3920283778
H	-6.1639419537	-2.3067865224	-1.2602613484

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15 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.3265740399	0.1158640588	-0.6516982943
C	-1.3065017707	1.8979345666	-0.0500613464
C	-0.2418777716	2.4185311487	0.7159417715
C	-2.2011746969	2.8389223514	-0.6031489719
C	-0.0553628597	3.7931317057	0.8890489004
H	0.4643696996	1.7368552068	1.1909455818
C	-2.0254254707	4.2163845688	-0.4402308495
H	-3.0613088145	2.4944412027	-1.1796126959
C	-0.9487108787	4.6971469818	0.3086357316
H	0.7821726161	4.1609844472	1.4787231552
H	-2.7285041966	4.9147035844	-0.8904268608
H	-0.8115474369	5.7671985349	0.4457441916
H	-1.1880624817	-1.2249148317	-1.403836107
S	-2.3068125693	-0.863382069	0.9350851521
C	-3.2553745852	0.2716481648	2.0345763778
H	-3.9988433546	0.84634915	1.4792857164

H	-3.7324105306	-0.3161376335	2.8223561168
H	-2.5312257472	0.9632408051	2.4659244333
Si	-3.9021827247	-2.0516122242	-0.0569396915
C	-3.0628342236	-3.6029418847	-0.6984346337
H	-3.7855656106	-4.2171697032	-1.250936664
H	-2.2409267868	-3.3410894932	-1.3705044912
H	-2.6615003967	-4.2101630903	0.1204448259
C	-4.7057351855	-1.0502124943	-1.435866967
H	-5.5429045765	-1.6132180969	-1.8690569566
H	-5.1009395685	-0.0938481037	-1.0747789171
H	-3.9836317201	-0.8458291564	-2.2325595962
C	-5.1629961722	-2.4705126061	1.2880993679
H	-5.9214644696	-3.1459061115	0.871641466
H	-4.6942599925	-2.9840875787	2.1351509496
H	-5.6857576836	-1.5864984004	1.6688323053

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TS$_{10A-12B}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.4382978087	-0.6204954096	-0.3952820133
S	0.2113835084	-2.7296990051	-0.351745739
C	2.1811245866	-0.6033099255	0.2293386791
C	1.6539478549	-3.6809293226	0.2606198372
C	3.2913319234	-0.6197814052	-0.6366760172
C	2.4292558132	-0.3698250429	1.5957215478
H	1.3538533412	-4.7336922302	0.2413766477
H	2.5253813387	-3.5442072333	-0.3827611059
H	1.9157420709	-3.3999888037	1.2825600688
C	4.5869279029	-0.372048528	-0.1678400046
H	3.1488586445	-0.8342015428	-1.694377433
C	3.7203437405	-0.1213676826	2.0710532237
H	1.6054599348	-0.386087305	2.3070191871
C	4.8018204285	-0.1203455335	1.1891017333
H	5.4267410303	-0.3829498552	-0.8595495613
H	3.8825384993	0.0638068573	3.1308957027
H	5.8083471484	0.0639112052	1.5565831568
Si	0.6202370704	3.1613417076	-0.1460253458
H	-0.1756475428	2.1733520434	0.649537653
C	2.2212042629	3.5453143194	0.7785063878
C	0.9767091592	2.3837135674	-1.8371467507
C	-0.4222948351	4.7303499832	-0.3406863172
H	2.7985650728	4.3133721278	0.2481309838
H	2.0191958316	3.9238001937	1.787675965
H	2.8513372684	2.6539491745	0.8729273492
H	1.7909263334	2.9010418103	-2.3579537518
H	0.0902662764	2.4016528461	-2.4818644334
H	1.2802161991	1.3343454056	-1.7216155237
H	-0.6493014033	5.1783394462	0.6340516892
H	0.1080114067	5.4840026476	-0.9360789081
H	-1.3747705191	4.52165755	-0.8420402675
S	-1.624464781	-0.0505140008	-1.2026044886
C	-2.9133827602	-0.1868908627	0.0486523042
C	-2.181914035	-1.2695353108	-2.4497967632
C	-3.8553789385	0.8441471393	0.1370632576
C	-2.9684447457	-1.2795833359	0.9215192871
H	-2.1207976655	-2.2805296037	-2.0420543411
H	-3.2001567349	-1.023140191	-2.7577569679
H	-1.5034665149	-1.183139868	-3.3017811886
C	-4.8646309133	0.7768007668	1.0992347466

H	-3.7948210503	1.6900651464	-0.5411249607
C	-3.9860026154	-1.339911272	1.875117424
H	-2.2208616045	-2.0660113176	0.8555534524
C	-4.9317009299	-0.3155537586	1.9661717001
H	-5.5956849892	1.5774164323	1.1701228801
H	-4.0334014674	-2.1875116667	2.5532556722
H	-5.7176634101	-0.3667003572	2.7147573461

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12B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.3175914528	-0.0539832893	-0.5123700995
S	-0.1866405723	-1.4497199907	-2.08298321
C	1.9999443489	-0.8334347775	-0.2222778091
C	0.9962731549	-2.8267858856	-2.3394819021
C	3.1189316225	-0.5363605232	-1.0204196929
C	2.2052396151	-1.6774545097	0.8844628315
H	0.5336278148	-3.4960496833	-3.0716736253
H	1.9503352149	-2.4701596437	-2.7328410456
H	1.1788718252	-3.3770947664	-1.41407862
C	4.3908627543	-1.0335940904	-0.7133864444
H	3.0002718272	0.0795370504	-1.9101456655
C	3.471362443	-2.185565104	1.1918071411
H	1.3669946739	-1.9472141071	1.5248196831
C	4.5730868099	-1.8603683542	0.3969183189
H	5.2373269481	-0.7816564608	-1.3492760316
H	3.5975202754	-2.8353714105	2.0556239111
H	5.5585670661	-2.2528845063	0.6351272975
Si	1.2543230585	2.1287452892	0.9900389335
H	0.4751864102	0.7946943259	0.8949038572
C	2.768219471	1.7548847645	2.0382197432
C	1.7113159232	2.9395717899	-0.6501574389
C	0.0069625732	3.2185795297	1.8982918703
H	3.2909670309	2.6863794681	2.2907708113
H	2.4917194265	1.2615307646	2.9765863471
H	3.4638800973	1.100317254	1.5055754309
H	2.1878039778	3.9065755113	-0.4373233806
H	0.8313868142	3.1370398391	-1.2714920036
H	2.4195002459	2.3372910783	-1.2254163211
H	-0.3059100445	2.7729907851	2.8493943836
H	0.4416071962	4.2020412423	2.1175285121
H	-0.8880977656	3.3763734094	1.2865452117
S	-1.7448149005	1.0739997299	-0.7010647157
C	-2.8907975322	0.2568812337	0.4237579671
C	-2.567239676	0.8119917807	-2.3145934552
C	-3.6889490968	1.049014548	1.2563908537
C	-2.9739344296	-1.1399455397	0.4754299759
H	-2.5700005637	-0.248129502	-2.5724549351
H	-3.579734287	1.2167349618	-2.2575625442
H	-1.985025511	1.3603003109	-3.0586240205
C	-4.5792257052	0.4399303981	2.1430880492
H	-3.6126776489	2.131211561	1.2080043183
C	-3.8738863178	-1.7379055145	1.3589512632
H	-2.3397292332	-1.7413505614	-0.1714518683
C	-4.6735155558	-0.9521649585	2.193047897
H	-5.1988082551	1.0537785685	2.7910860554
H	-3.9441011641	-2.8214449382	1.3992766802
H	-5.3678188124	-1.4245090773	2.8826984852

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$TS_{12B\text{-}16A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.2215632032	0.0659202171	-0.4091422622
S	-0.3997279528	-1.5397505533	-1.8221080282
C	1.9409999633	-0.8066665488	0.0056773264
C	0.878142201	-2.806989107	-2.1634556058
C	3.0736914993	-0.5856995443	-0.7976330866
C	2.0005522165	-1.8277331721	0.9711903974
H	0.4370885166	-3.5174427418	-2.8688840871
H	1.7699999662	-2.3675763627	-2.6173887642
H	1.1723559964	-3.3436519324	-1.2583371873
C	4.2035114787	-1.397579757	-0.6832003445
H	3.0673251772	0.2185363697	-1.5297243576
C	3.1311827952	-2.6371572533	1.0881368962
H	1.1516366494	-1.9997136897	1.6282846201
C	4.2358785476	-2.4286614064	0.2582614111
H	5.0612313286	-1.2215635364	-1.3279003913
H	3.1509452792	-3.4309556288	1.8310388283
H	5.1180416774	-3.0561904161	0.3528541004
Si	0.8721595886	2.115093514	0.7609325824
H	1.3834200258	0.3625579635	0.4968940612
C	2.6321047874	2.2901084453	1.4634197667
C	0.7555839775	3.4129968852	-0.6240844961
C	-0.3222209825	2.479887641	2.1906162869
H	2.7946126562	3.3159150466	1.819489299
H	2.812157996	1.6119150442	2.3055335167
H	3.393014634	2.0765679931	0.7041766558
H	1.0017084356	4.4012245452	-0.212051109
H	-0.238129576	3.4746719689	-1.0774801025
H	1.4827998923	3.1988561623	-1.4161661481
H	-0.176813087	1.760197021	3.0047672639
H	-0.1136157682	3.4799591682	2.5936688076
H	-1.3750816918	2.4495715151	1.8970939321
S	-1.8338328105	1.0855864918	-0.6115451771
C	-3.0267634678	0.2392768693	0.4471962507
C	-2.5676765586	0.8326501067	-2.2719606919
C	-3.9266989028	1.0338521237	1.1679808756
C	-3.0648905007	-1.1554522338	0.5522708759
H	-2.5327427522	-0.2205033915	-2.5518503764
H	-3.5891770812	1.2185813755	-2.2480338899
H	-1.963259102	1.4133033328	-2.9724617908
C	-4.8708413641	0.4287477836	1.9993768683
H	-3.8877801279	2.1153018176	1.0756675064
C	-4.0176821563	-1.7492080118	1.382439845
H	-2.3639441623	-1.7586158009	-0.0206681345
C	-4.9164683416	-0.9625837337	2.1069365198
H	-5.5684287486	1.044766035	2.5600660107
H	-4.0535107484	-2.8321966888	1.4635477233
H	-5.6514451058	-1.4329003961	2.7546143932

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16A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.4251906017	0.2105717858	-0.3983017166
S	-0.1503917622	-1.3902383833	-1.8947033092
C	2.2814405165	-0.7955392127	0.1024775097
C	1.0526378465	-2.7402002562	-2.1876053801
C	3.3704551191	-0.6393988774	-0.7658205353

C	2.2253759879	-1.9086165879	0.9534490586
H	0.6193739832	-3.3929987172	-2.9511704505
H	2.0078618043	-2.3588834489	-2.5574849017
H	1.2349650762	-3.3315732895	-1.2869331775
C	4.3576767938	-1.6225948847	-0.8322029477
H	3.4394826761	0.2450819331	-1.3924598945
C	3.2152565898	-2.8879928587	0.8874276289
H	1.407159724	-2.0084420937	1.660917107
C	4.2806586741	-2.7475621615	-0.0069917241
H	5.1921494654	-1.5067880866	-1.5184990524
H	3.1631976573	-3.7557796596	1.5394528266
H	5.056138135	-3.5075243391	-0.0512975817
Si	0.9697123231	2.2147682446	0.7229066839
H	1.7643819969	0.1634780713	0.4732859099
C	2.7620635946	2.3179139715	1.3822674997
C	0.846525061	3.6253688871	-0.5575305538
C	-0.1414327624	2.6035891069	2.2232749698
H	2.9475528941	3.3195012876	1.7929871809
H	2.9587381165	1.5918319277	2.1800973286
H	3.5046041738	2.1459180426	0.5938740403
H	1.0950200881	4.583282599	-0.0803077281
H	-0.1526850247	3.7198542592	-0.9955379345
H	1.5615183881	3.471154121	-1.3749758461
H	0.0053746999	1.8625367961	3.0182496053
H	0.1219162917	3.5869091773	2.6359452074
H	-1.2070718126	2.6209367948	1.9752956815
S	-1.5946342362	1.1693998727	-0.5801086421
C	-2.7660262685	0.2582291096	0.4514891509
C	-2.3260516389	0.9481476833	-2.2479935841
C	-3.6478378096	1.013529696	1.2336355541
C	-2.8110988323	-1.1398061833	0.4717856853
H	-2.2666296677	-0.0935474267	-2.5633313175
H	-3.3565263035	1.3075818507	-2.201863127
H	-1.741065618	1.5697611371	-2.9294495041
C	-4.5813783543	0.3643879066	2.0435936277
H	-3.6041003925	2.0982000015	1.205241257
C	-3.7540434818	-1.7769681227	1.2804966742
H	-2.122414934	-1.708472774	-0.1499879451
C	-4.6346245949	-1.0305220326	2.067469486
H	-5.2649567937	0.9493561281	2.6526742919
H	-3.7967576846	-2.8626959925	1.2959319821
H	-5.3615583062	-1.5350180023	2.6983359065

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TS$_{10A-12C}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.3778081368	-0.8699205013	-1.113890295
S	-1.6576244461	-2.5781500738	-1.4812776327
C	0.0194912661	0.943504035	-0.8110022659
C	-1.8454790208	-3.4710544505	0.1151336674
C	-0.056875676	1.8843143573	-1.8547149491
C	0.2677788175	1.4370353409	0.4829813376
H	-2.5292468163	-4.3109849556	-0.0338914532
H	-0.8796975666	-3.8668189751	0.4472497223
H	-2.2496886933	-2.8201258956	0.8957546719
C	0.0846943604	3.2563243985	-1.6155392858
H	-0.2338554253	1.5526678086	-2.8773887744
C	0.4116937939	2.8065861114	0.7303337176
H	0.3388958078	0.7478207715	1.3240900724

C	0.3196150352	3.7224054913	-0.3205231147
H	0.0128262625	3.9599723701	-2.4422795794
H	0.5952980876	3.1580412228	1.7437140495
H	0.4340229484	4.7869414101	-0.1323957894
Si	-3.5555351482	0.3485139576	0.8157150258
H	-2.2327649434	-0.3514058518	0.7748530304
C	-3.4780693276	1.6665090527	2.1744440519
C	-3.8865451737	1.1403056264	-0.8671994365
C	-4.8880553317	-0.9353581085	1.2193914779
H	-4.4214760994	2.2224990868	2.2440743424
H	-3.2850323814	1.2174802085	3.1564000356
H	-2.6778292845	2.3877477804	1.9722133701
H	-4.8470060672	1.670971597	-0.8708676729
H	-3.9196638103	0.378092209	-1.6541100381
H	-3.1013179546	1.8589778939	-1.1270256848
H	-4.7128539899	-1.4053476302	2.1947287891
H	-5.8842752371	-0.4761935071	1.2474966178
H	-4.9083020069	-1.7285438293	0.4631410726
C	2.3272720831	-2.7648250279	0.730925415
C	2.0845493078	-2.8452511499	-0.644771985
C	2.7018226409	-3.9119009511	1.4319806677
C	2.1889647338	-4.0694345993	-1.3122652485
C	2.8152339354	-5.1359911744	0.7683468911
H	2.8954130947	-3.8489795565	2.4991478155
C	2.5533721583	-5.2136359415	-0.6008666382
H	1.9816522023	-4.123270878	-2.3763299211
H	3.1021630257	-6.0274490446	1.3188019177
H	2.6347913318	-6.1643340107	-1.1199111837
H	2.2249669191	-1.8189819805	1.2544309757
S	1.6042874044	-1.4084236302	-1.6211191212
C	2.9172943172	-0.2229746965	-1.1567567215
H	2.7488356089	0.6750324544	-1.7527266025
H	2.8717945436	0.0435942911	-0.1004545038
H	3.8804525207	-0.6744045753	-1.4057373072

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12C B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.231677257	0.6899070651	0.1784927414
S	-2.3683554786	1.4307340277	0.2716059276
C	1.4969377625	-0.1379032637	0.2816628923
C	-2.8337811879	1.3757045095	2.050487985
C	2.5057734239	-0.1059993367	-0.6973770346
C	1.7534172209	-0.916618247	1.4268664517
H	-3.8658616039	1.7283232759	2.135600318
H	-2.7860775785	0.3578815034	2.4494711912
H	-2.1990813385	2.0218555274	2.6643681583
C	3.7110931775	-0.8006164408	-0.5420842528
H	2.3586450116	0.4671970808	-1.6113452461
C	2.9453444826	-1.6289785823	1.5852612361
H	1.0139747127	-0.9703536748	2.2252920201
C	3.934252565	-1.5696057386	0.6008163684
H	4.471619684	-0.7444036918	-1.3183473494
H	3.1054838113	-2.2240815796	2.4819790899
H	4.8670655884	-2.1143010469	0.7241798566
Si	0.7876010289	2.7498943447	1.1372078038
H	0.0487867448	1.3808264017	1.5281310618
C	2.4519823418	2.5813403163	2.0057233082
C	1.0110237752	3.3678595184	-0.6373245052

C	-0.3083449238	3.9815170865	2.0543440723
H	2.9109791474	3.5734088339	2.1093092597
H	2.3411287233	2.1604871365	3.0113932876
H	3.1360781295	1.9384219938	1.445877579
H	1.4811268634	4.3605787489	-0.586779362
H	0.0494419842	3.4797088346	-1.1470681937
H	1.6604065247	2.722134564	-1.234356431
H	-0.4490764209	3.7168647605	3.1080938186
H	0.1588828007	4.9746041791	2.0237279615
H	-1.2903534423	4.0485480584	1.5764830708
C	-2.1143348107	-2.3390615222	-0.500543837
C	-0.9488496213	-2.1008572598	-1.2378480124
C	-2.4324546125	-3.6472221779	-0.1334273726
C	-0.0966803587	-3.1515375274	-1.5882236812
C	-1.587693415	-4.7042594347	-0.482735214
H	-3.3385111708	-3.8383962071	0.4351454421
C	-0.4191954411	-4.4547494937	-1.2041652782
H	0.8106477731	-2.9484910288	-2.1481030443
H	-1.8387058734	-5.7199532747	-0.189409069
H	0.2429768705	-5.27304435	-1.472916136
H	-2.7511795181	-1.5072715668	-0.2115986275
S	-0.4946739894	-0.4353955472	-1.7556068649
C	-1.9893311876	0.0568187329	-2.6887674811
H	-1.7711379875	1.0282354395	-3.1399149257
H	-2.1604534999	-0.6844881668	-3.4725217233
H	-2.8512854304	0.1524752202	-2.0270152599

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TS$_{12C-16B}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	1.0831076813	0.691616861	-0.1177294123
S	-0.6713918501	2.0956123936	-0.3218929712
C	2.6269395366	-0.4751769761	0.1187816954
C	-1.9031458356	1.2868138561	0.7766954989
C	3.630609909	-0.5383931866	-0.863934755
C	2.6843373473	-1.3995382307	1.175887958
H	-2.849929102	1.8260601363	0.6767052249
H	-2.0783858717	0.2377614639	0.5117714034
H	-1.5959834383	1.329746655	1.8265827656
C	4.6196045202	-1.5245746836	-0.8237640955
H	3.636927026	0.1834120356	-1.6781892905
C	3.6707006375	-2.3873432222	1.219727213
H	1.9455762398	-1.3566808376	1.9739070336
C	4.6407479296	-2.4551501627	0.2174488811
H	5.3776057253	-1.5618297632	-1.6029167989
H	3.6852047779	-3.1008338185	2.0402738598
H	5.413909275	-3.2182771634	0.2543705629
Si	1.938344554	2.5841173145	1.1704292203
H	2.3210105238	0.9504393819	0.6379669513
C	3.6992558499	2.3942421544	1.8989741132
C	2.0872014295	4.0227502513	-0.0490367019
C	0.8368116458	2.8768108057	2.6806022409
H	3.9875043046	3.3197885998	2.4155859417
H	3.7621525307	1.5749904121	2.6250653795
H	4.4476674247	2.2001629227	1.1215998281
H	2.4803605345	4.8986255644	0.4845599549
H	1.1339182487	4.2903264535	-0.5091033133
H	2.8052563775	3.7758347791	-0.8403965168
H	0.7654365549	1.971543623	3.2956572299

H	1.2938646319	3.6560001693	3.3050081699
H	-0.170168061	3.1942948843	2.4030358634
C	-0.4906542759	-2.9984371728	-0.0703788065
C	0.3124378699	-2.5479554815	-1.1252878617
C	-0.4460734082	-4.3385026206	0.3128257711
C	1.1728500591	-3.435076711	-1.7783290975
C	0.4117615734	-5.2275023184	-0.3406810273
H	-1.0741461826	-4.6859389729	1.1286964114
C	1.2229972215	-4.7730852653	-1.3808376001
H	1.8013582741	-3.0767220033	-2.5869958936
H	0.4486180022	-6.2699035385	-0.0364492528
H	1.8946444342	-5.4592250053	-1.8893062682
H	-1.1449719783	-2.3049156629	0.4506823552
S	0.2815626374	-0.8290158927	-1.6535960772
C	-1.4559877452	-0.671092676	-2.2005898541
H	-1.6318171784	0.3962820099	-2.3472175099
H	-1.5794138602	-1.2217186919	-3.1356373268
H	-2.1467680103	-1.0528678395	-1.4470097065

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16B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0041070591	1.2213246454	-0.0219920532
S	-1.8884667593	2.2982497367	-0.1259065996
C	1.7640478185	-0.0346571318	0.271550128
C	-2.9515622539	1.2333451534	0.9309693061
C	2.3894480636	-0.7681730775	-0.746544818
C	1.6865571739	-0.5668591062	1.5663105893
H	-3.9718880507	1.6248952475	0.8752779306
H	-2.9616096015	0.1898796074	0.5962345527
H	-2.6300719688	1.2638627657	1.9765629391
C	2.8699262631	-2.0509773387	-0.487999523
H	2.4908546609	-0.3359501024	-1.7375706673
C	2.1535858675	-1.858099342	1.8172032034
H	1.2700966099	0.0265868555	2.3743369158
C	2.7438429134	-2.5996314232	0.7913554396
H	3.3461345025	-2.6217210384	-1.2802431594
H	2.0734572852	-2.2786109392	2.8158593506
H	3.1192258081	-3.599474142	0.9917358944
Si	0.5433880275	3.0523880399	1.2065089613
H	1.6541241708	1.0757750236	0.1189247299
C	2.4120418261	2.9687910637	1.6731517759
C	0.4072152147	4.7141275604	0.2872565677
C	-0.3376488406	3.1416605027	2.8951358119
H	2.6657710566	3.8568856363	2.2686406147
H	2.678574899	2.0891647341	2.2701800673
H	3.0609803137	2.9745931511	0.7881763165
H	0.8104799946	5.5181233161	0.9180241023
H	-0.6250900151	4.9619905545	0.0271172406
H	0.9978586651	4.6977226345	-0.6372406917
H	-0.2167704316	2.2107586303	3.4643436357
H	0.0990853876	3.9485515184	3.4992535295
H	-1.4086163918	3.3381430968	2.7876848509
C	-1.2221840315	-2.697335651	-0.0065080097
C	-0.7621776117	-2.2759253647	-1.2599955607
C	-1.251239155	-4.058029801	0.3045906379
C	-0.3209403848	-3.2229470915	-2.1927979565
C	-0.8184217643	-5.0014075789	-0.6295379941
H	-1.6105573118	-4.3796105585	1.2784318739

C	-0.3531498087	-4.5823626899	-1.8778732695
H	0.0437366777	-2.8914054082	-3.1604616988
H	-0.8422698837	-6.0598799096	-0.384888157
H	-0.0139674756	-5.312894696	-2.6074601302
H	-1.5529771884	-1.9624573707	0.7211972344
S	-0.7257613883	-0.5286856676	-1.6855370651
C	-2.4191113616	-0.318975366	-2.3485775156
H	-2.5863665255	0.7569221641	-2.4305740097
H	-2.492056754	-0.8000174925	-3.3264125324
H	-3.154587183	-0.7455083506	-1.6633447888

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TS$_{12C-13B}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.5030407669	0.079017482	-0.2227223255
S	-0.6210513933	1.9942046093	-0.6185314767
C	1.8007278816	-1.3007692797	-0.1311578488
C	2.3647666407	-1.8671783661	-1.2910674715
C	2.2541655341	-1.8103948138	1.102086925
C	3.3103821248	-2.8950652646	-1.2274859164
H	2.0663084917	-1.5004800574	-2.271825282
C	3.2045236233	-2.8358873132	1.1766208035
H	1.8551410249	-1.4117939305	2.0344527793
C	3.7357984495	-3.3858442941	0.0092788018
H	3.721807892	-3.3087540845	-2.1462191152
H	3.5275084527	-3.2044100924	2.1483879198
H	4.4738538633	-4.1824914549	0.0616899212
C	-1.6335147174	2.5608828288	0.8074379707
H	-1.0139110773	2.7287001422	1.692756542
H	-2.112395479	3.5034237437	0.5305375732
H	-2.4051787909	1.824470451	1.0445045438
H	1.611962631	0.8607483782	-0.8564717207
Si	1.8127750829	2.3771910189	0.0056448044
C	1.4956850388	4.2536545796	-0.1370153596
H	2.3814588444	4.8082737131	0.2038379336
H	1.3028835779	4.5379063905	-1.1776699931
C	1.9947501365	1.9388168545	1.8419067209
H	1.0459090392	1.909072952	2.388016897
H	2.6200641542	2.7106690426	2.3109767335
C	3.5274761633	2.2098069979	-0.8236053954
H	4.215409174	2.962503083	-0.4152224761
H	3.9510440401	1.2128037977	-0.6644111357
H	0.6337011283	4.5765089236	0.4563825521
H	2.494863363	0.9742348897	1.9690682916
H	3.4643655332	2.3756098208	-1.9062874857
S	-1.0751110922	-1.2705232168	0.6451833536
C	-2.7643623954	-0.8559157487	0.1795582172
C	-0.9602136177	-2.9491393211	-0.0807128711
C	-3.102421901	-0.5354436947	-1.1407290337
C	-3.7480143007	-0.866709271	1.1756058107
H	-1.743642592	-3.5689992928	0.3602676327
H	-1.0692077847	-2.9106091355	-1.1662478583
H	0.0262870181	-3.335806665	0.1750547571
C	-4.4282764459	-0.2421492432	-1.4618289939
H	-2.3333162611	-0.5009663549	-1.9049689476
C	-5.0719599131	-0.5657257179	0.8476029815
H	-3.4762247257	-1.1131340109	2.1978681368
C	-5.4125581602	-0.2561709507	-0.4703399804
H	-4.6894253306	0.0069568215	-2.4864738863

H	-5.8341804536	-0.5755958168	1.6217682769
H	-6.4426712382	-0.0224301292	-0.7247223059

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13B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.6626803286	-0.0359065876	-0.1821432221
S	-0.1123770144	2.0967326208	-0.3277433402
C	1.6617268774	-1.6187785895	-0.3088588987
C	1.4709586791	-2.5464241071	-1.3531652606
C	2.6036383157	-1.9764675336	0.6776466634
C	2.1505167334	-3.768364711	-1.3955237251
H	0.7780337183	-2.3150773942	-2.1616179071
C	3.2859399467	-3.197297784	0.6465185097
H	2.8169805743	-1.2887508685	1.4957066122
C	3.0608222602	-4.1043947205	-0.3911429593
H	1.9717927561	-4.4580170708	-2.2189466901
H	4.0011441814	-3.4372747183	1.431726191
H	3.59249014	-5.0525420324	-0.4215889138
C	-1.3791035193	2.6096087179	0.9111749054
H	-1.0504573111	2.410214913	1.9339035155
H	-1.6041619979	3.6708609222	0.7888343896
H	-2.2798665821	2.0273322784	0.7073920503
H	1.8226144125	0.4462009106	-0.9324533787
Si	1.6437085394	3.3159502057	0.2316246431
C	1.0097805451	5.0529115582	0.6309152142
H	1.8649796197	5.716843257	0.8117660568
H	0.4353180166	5.4730092633	-0.2024964436
C	2.5257976178	2.576081112	1.7241846815
H	1.8561128652	2.4614828731	2.5843371159
H	3.3555469643	3.2258228528	2.0325560986
C	2.7510001162	3.3536315136	-1.2865376198
H	3.6571221455	3.9344988048	-1.0706352407
H	3.0514278825	2.3425986353	-1.5761024591
H	0.3818577117	5.0789962766	1.5282689867
H	2.9347248399	1.5912868827	1.4767900592
H	2.2465092156	3.8210523587	-2.1393579687
S	-1.0446036608	-0.9164338828	1.0443265092
C	-2.5954957652	-0.8577074337	0.1294071984
C	-0.8762153766	-2.7252377743	1.2766557697
C	-2.5959974035	-0.6829621057	-1.2596284294
C	-3.8089947536	-0.9623806608	0.82207741
H	-1.738297487	-3.0931405322	1.8370686892
H	-0.784093589	-3.2259875186	0.3120315497
H	0.0436424396	-2.8834910226	1.8423504702
C	-3.8070461989	-0.624162524	-1.9521728706
H	-1.6511144305	-0.5911380476	-1.7858562608
C	-5.0156032529	-0.9121230347	0.1227995843
H	-3.8047654634	-1.0806632164	1.9020290166
C	-5.0160349518	-0.7422379995	-1.2641032174
H	-3.802708133	-0.488371506	-3.0301151885
H	-5.9548993103	-0.9976219172	0.6624457886
H	-5.9569632415	-0.698485663	-1.8056726845

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TS_{16B-17} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.1806862062	-0.4307352321	-0.1225932341
S	-1.9305388161	-2.0929304549	0.9720296257

C	0.3888022723	2.0233814248	-0.1143037748
C	0.8714900696	2.1565269232	1.1891064684
C	1.0963363682	2.564570948	-1.1902061169
C	2.0754907838	2.8268116093	1.415392886
H	0.3118581788	1.7380599591	2.0205326708
C	2.2984848723	3.2373769681	-0.9604363498
H	0.7100300179	2.4650479286	-2.2005597598
C	2.7877784051	3.3670144062	0.3419095634
H	2.4558969733	2.929623806	2.4279533691
H	2.8496189015	3.6638787833	-1.7944564515
H	3.7226992507	3.8917037282	0.5206527916
C	-2.8312314408	-3.1932747387	-0.1969955885
H	-3.063874436	-4.110619264	0.352581368
H	-3.7699819627	-2.7409554695	-0.5246793427
H	-2.2374070566	-3.457914429	-1.0763582232
H	-0.5790369927	1.5478716065	-0.2937204308
Si	-3.0852980402	0.6342119325	0.3271458583
C	-3.1471550389	2.140573341	-0.8739122146
H	-3.1418605727	1.8226354203	-1.9243865249
H	-4.0885455484	2.6822221599	-0.7047655314
C	-4.7494022512	-0.2344774394	0.0057658824
H	-4.9207521198	-1.0642526607	0.6985110361
H	-5.5671085577	0.4878044816	0.1340814913
C	-3.1291192017	1.3208752414	2.1050646165
H	-4.0381273222	1.9159121478	2.267766793
H	-3.124265501	0.5030564392	2.8338823174
H	-2.3282265643	2.8543355177	-0.7347763636
H	-2.2703380014	1.9696379432	2.3166876278
H	-4.8173519667	-0.6209249785	-1.0186645686
S	0.7893107033	-1.0364201432	-1.3895254394
C	2.1736185359	-1.2119220351	-0.2529183335
C	0.5207283492	-2.7775121029	-1.8805943734
C	2.0282935045	-1.9142207301	0.9504872918
C	3.3955370568	-0.6166754462	-0.5824526529
H	1.4437949109	-3.1854402564	-2.2979837575
H	0.1887022373	-3.3669884194	-1.0230654924
H	-0.2575515044	-2.7750062522	-2.6481755517
C	3.1199454257	-2.0328648508	1.8115547948
H	1.0687489555	-2.3531059743	1.2109198359
C	4.4777957728	-0.7300542145	0.2925281181
H	3.4930047912	-0.066425654	-1.5128313707
C	4.3434833261	-1.441791124	1.4858417028
H	3.0093394584	-2.580507131	2.7435784928
H	5.4265387645	-0.2661677554	0.0367530547
H	5.1889402458	-1.5336223599	2.1622961404

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$TS_{16B\text{-}18A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.2559367256	0.2614650907	-0.1286226624
S	-1.8524196355	-1.7408263919	0.2341133797
C	-0.085640615	1.9461046313	-0.4799490835
C	0.5683185904	2.3900282721	0.6802953476
C	0.5609394241	2.0341562464	-1.7230968485
C	1.8860050358	2.8401870193	0.60731334
H	0.0484991672	2.3802282562	1.6336592284
C	1.8745401096	2.4941532251	-1.7921788695
H	0.0401106976	1.7351951289	-2.6277387018
C	2.5383046835	2.8905421341	-0.6270029171

H	2.4012958535	3.1588289146	1.5088240583
H	2.3794550888	2.5487842409	-2.7524764435
H	3.561496336	3.2518561638	-0.6836165179
C	-2.527596899	-2.2981143083	-1.3878013441
H	-2.7482925229	-3.3662462277	-1.3039366333
H	-3.4560336532	-1.7727649527	-1.6278333296
H	-1.8127810676	-2.150972028	-2.2021587895
H	-1.2158222661	1.8805139746	-0.479421108
Si	-3.1647946108	0.8633924785	0.8564551949
C	-3.2699206912	2.7802355555	0.7974711321
H	-3.3372568341	3.1647064705	-0.2277487677
H	-4.1749701824	3.1046544019	1.3299263579
C	-4.7679992178	0.2653048286	0.0284873012
H	-4.9042835104	-0.814308019	0.1428665668
H	-5.6293031325	0.7701375962	0.4866367852
C	-3.173628387	0.4212395694	2.7058646961
H	-4.0662488006	0.8444215615	3.1867932123
H	-3.1762205154	-0.6615356612	2.8619030749
H	-2.4150051083	3.2701871221	1.2786967006
H	-2.2974062613	0.8361812524	3.2191939144
H	-4.7845292807	0.5021126535	-1.0424211987
S	1.5366132819	-1.3201914013	-1.7122323863
C	2.5583585923	-1.1841274595	-0.242139995
C	1.0921384434	-3.0959400245	-1.6666949969
C	2.0681905547	-1.5328565934	1.0247133153
C	3.861817278	-0.686558995	-0.3672117373
H	1.9887073879	-3.7124037035	-1.5664347448
H	0.3902681549	-3.2954716278	-0.8528137258
H	0.6074205017	-3.3205650819	-2.6212166572
C	2.8852240916	-1.398071501	2.1481280915
H	1.0522066097	-1.9025204087	1.1270733495
C	4.6666763455	-0.5355346258	0.7640008855
H	4.2427447642	-0.4278845456	-1.3506330802
C	4.1829764515	-0.8954190996	2.0230000351
H	2.5011288669	-1.677987016	3.1257319844
H	5.6775462354	-0.1502136917	0.6571477523
H	4.8137687214	-0.7880609743	2.9014612846

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17 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.692554373	-0.0810130152	0.0631293913
S	1.2479244872	0.9302689878	0.0769991071
C	2.4074056863	-0.3211215804	-0.518370674
C	3.7094860686	0.06556628	-0.8556430626
C	1.9993016044	-1.6488265073	-0.6797569015
C	4.6108411972	-0.8867468196	-1.3317835348
H	4.0113206464	1.1041890026	-0.7523220439
C	2.9039151161	-2.593214563	-1.1677895165
H	0.9793933196	-1.9402849082	-0.4389465658
C	4.2089924184	-2.2159467366	-1.4886164998
H	5.6227693273	-0.5879975808	-1.5909776671
H	2.5842998643	-3.6233864322	-1.2966256122
H	4.9107563439	-2.9537790768	-1.867380823
C	1.8282127835	1.1196596696	1.8105650624
H	1.7618400453	0.1741664125	2.3524035425
H	2.8594315872	1.4789861252	1.801960538
H	1.1845143166	1.8652187918	2.2818346461
S	-2.1733425573	-1.5494258695	-0.1807997791

C	-2.6235498852	-2.1864852607	1.4913043817
H	-3.2520356609	-3.0695698263	1.3457346844
H	-1.7478551949	-2.4752334883	2.0784348298
H	-3.1979544658	-1.4413754382	2.0482082543
Si	-2.0826366033	1.6393988076	0.2248402743
C	-1.171588595	3.2243584874	0.7984644384
H	-1.87092056	4.0714999044	0.7622394121
H	-0.819341189	3.1452328878	1.834984986
H	-0.3139361828	3.4771715301	0.164848736
C	-3.492569898	1.4126743839	1.4809914639
H	-4.0595936915	2.3485299247	1.5808126344
H	-4.1853542103	0.6260815262	1.1652671132
H	-3.1138200752	1.1531531038	2.4772218248
C	-2.8229135845	2.0211215381	-1.4847933271
H	-3.415596425	1.1768580444	-1.8518145287
H	-3.4755091553	2.9034560151	-1.4288574538
H	-2.0414875052	2.2321036799	-2.2243933309

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$TS_{17\text{-}19}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.1737686217	-1.4180371281	0.0614892982
S	2.006207566	-0.5098377977	-0.2974953956
C	3.2104246167	-1.7764322343	-0.7682795766
C	4.4891984614	-1.4332025486	-1.2195990309
C	2.8108891239	-3.1165390192	-0.7448762708
C	5.373484557	-2.4360491126	-1.6203152431
H	4.7904670754	-0.3900037804	-1.2651009686
C	3.6938454211	-4.1139909589	-1.1588764479
H	1.8016393647	-3.3381634852	-0.4079403877
C	4.9780518364	-3.7763895168	-1.5914106296
H	6.3687197901	-2.1695802504	-1.9666523956
H	3.3796276694	-5.1542157088	-1.139737954
H	5.6679881626	-4.5529949423	-1.9104116424
C	2.8640067784	0.1734523406	1.1912251271
H	3.0059877428	-0.5946285519	1.9543207991
H	3.8288335455	0.594393223	0.8979178513
H	2.2268838002	0.9694001458	1.5848781333
S	-1.7503473604	-2.2181229433	0.0866400769
C	-2.2927536891	-2.9760245114	1.6975487131
H	-3.3773195664	-3.1033989878	1.6778389204
H	-1.8113883075	-3.9528200376	1.7769087691
H	-2.0035309732	-2.3655982167	2.5558055441
Si	-2.2905434875	-0.0576232997	0.3081889759
C	-1.4112060987	0.9236614158	1.6725205333
H	-2.0119059901	1.7993486751	1.9585850223
H	-1.268803789	0.3168022534	2.5739913179
H	-0.4267383219	1.2669583484	1.3422822278
C	-4.1243306757	-0.1066764298	0.8093541548
H	-4.5199736172	0.9154676441	0.8791801692
H	-4.7324068432	-0.6517733426	0.0782969388
H	-4.2714109073	-0.5790092233	1.7880268146
C	-2.1662697577	0.7580773493	-1.3898704682
H	-2.5220117071	0.0788222113	-2.1725029603
H	-2.7977294585	1.6566315135	-1.4151735054
H	-1.1405627729	1.048139637	-1.6354684005

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19 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.2237876957	-0.0282657429	0.1883005835
S	1.6345911016	0.7819833739	-0.1853859882
C	2.7888237206	-0.5089199522	-0.7145091061
C	4.0619080059	-0.1945113319	-1.2019528081
C	2.3533978974	-1.838178616	-0.7006479071
C	4.9039396563	-1.2140793837	-1.6490392974
H	4.3913446404	0.8405122248	-1.2396565667
C	3.193416552	-2.8524843237	-1.1606261219
H	1.3498121533	-2.0349363078	-0.3336579807
C	4.4719442798	-2.5432660862	-1.6299192017
H	5.8946150809	-0.9691870097	-2.0234949024
H	2.8507156819	-3.8838700508	-1.1483521553
H	5.1288984517	-3.332981909	-1.9845692525
C	2.5550433122	1.4047250542	1.2948059523
H	2.6832805476	0.6191224311	2.0423948548
H	3.5294258396	1.79161917	0.9856724777
H	1.9583858371	2.2183917722	1.714746319
S	-2.2148751761	-0.6699375396	0.2357672648
C	-2.7824658552	-1.5366579521	1.7811051126
H	-3.8586957256	-1.7152689915	1.719037427
H	-2.2583820924	-2.4936440889	1.8186232735
H	-2.5459816158	-0.9639513935	2.6805444195
Si	-3.2033789198	1.2966888929	0.3888007508
C	-2.5409791918	2.2989200849	1.8455815142
H	-3.0734258696	3.2561268505	1.928260358
H	-2.6617314513	1.769807426	2.7980519449
H	-1.4741935397	2.5025554843	1.7079399006
C	-5.0636102655	1.0146677975	0.5963549073
H	-5.5883768121	1.9789701351	0.6018792643
H	-5.4706490666	0.4166726785	-0.2266387883
H	-5.3043463085	0.5061508729	1.5369838459
C	-2.843069281	2.1607707739	-1.2449381666
H	-3.2327607697	1.5892507749	-2.0946512939
H	-3.311595148	3.1534563774	-1.261243946
H	-1.7649759741	2.2842995045	-1.3878126879

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18A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.3382812189	0.0333814248	-0.0689639664
S	0.5023921331	1.979866557	-0.5001444121
H	-0.9494542282	-2.5356031809	-1.0155815506
Si	1.796178173	-0.6022368612	-0.0752478914
C	2.9156792988	0.1761195382	1.2500089667
H	2.4629941096	0.1119076938	2.2475189522
H	3.8699340949	-0.3664728207	1.2922969609
C	1.8566287931	-2.4765496713	0.3458295949
H	1.2611142308	-3.1013851419	-0.3303477743
H	2.8991953959	-2.8131884081	0.2577409523
C	2.5947114885	-0.4724220983	-1.7950420617
H	3.6035536484	-0.907005401	-1.7741071526
H	2.0150223387	-1.0270590032	-2.543341878
H	3.127943143	1.2277722003	1.0375010364
H	2.671808991	0.5671242919	-2.1256166809
H	1.53885221	-2.6894995503	1.3738570785
C	-1.4325014656	-1.6906809177	-0.5374730048
C	-2.260715023	-0.8286983108	-1.2970694639
C	-1.3208091242	-1.5159624744	0.8657612497

C	-2.906149822	0.2333436571	-0.6688256134
H	-2.3651270141	-0.9817161455	-2.3661709849
C	-2.0031183276	-0.4444050411	1.4940732669
H	-0.7647250279	-2.2315290345	1.4597380102
C	-2.76638273	0.4338884519	0.7231234208
H	-3.4945488562	0.9332059693	-1.2529854018
H	-1.9231667866	-0.3060451508	2.567379603
H	-3.2540113899	1.2821973786	1.1927359308
C	0.4123380838	2.8517112979	1.1192969818
H	0.7564704585	3.8778942095	0.9595503119
H	-0.6091189266	2.8849589565	1.5101619055
H	1.06424935	2.3835785853	1.8629206146

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TS$_{18A-20}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.394056159	-0.5719147565	-1.0380517994
S	0.4914402757	1.3924980574	-1.3671941697
H	-1.8095712667	-2.4417939718	-1.9450314737
Si	1.7611302225	-0.5004755849	-0.6268520188
C	2.4962805236	0.0505623155	1.0289147729
H	1.7489813305	0.0099599501	1.8299977581
H	3.3147048844	-0.6244227823	1.3114948683
C	1.3088981937	-2.3857246687	-0.3560217679
H	0.6275609532	-2.8440116289	-1.0803155612
H	2.2665570726	-2.9149977296	-0.4687371387
C	3.0624362212	-0.4886557452	-2.0033679145
H	3.8607619295	-1.208697266	-1.7814488892
H	2.6207267844	-0.7719933542	-2.9660847135
H	2.900159064	1.0675156301	0.9867129204
H	3.5153485613	0.5003594175	-2.1228553235
H	0.9313645704	-2.5882018855	0.6507299296
C	-2.0065733186	-1.7101489485	-1.1611248992
C	-2.5184962802	-0.4166365968	-1.4882528335
C	-2.028698223	-2.1142025308	0.2024424851
C	-3.1717824879	0.3474144981	-0.4935803419
H	-2.619694684	-0.1227582705	-2.5289095397
C	-2.6246360465	-1.3176837957	1.1772459768
H	-1.6311634967	-3.0884503799	0.4726134851
C	-3.2268743534	-0.0972858129	0.8219196619
H	-3.6334777306	1.2918433676	-0.7700756739
H	-2.6445083443	-1.6542850724	2.2101650286
H	-3.7313623633	0.4984735996	1.5777500128
C	-0.0849631313	2.3558619603	0.0954257441
H	0.2415586921	3.3899997862	-0.0419989329
H	-1.1748511712	2.3194441322	0.167738183
H	0.3453330172	1.9680135963	1.0216191646

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20 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.1013402928	0.3280466718	0.1024176881
S	0.0094861688	-0.8645499113	1.9053633344
C	1.0504706845	1.5924587966	-1.2723089603
C	-1.732633363	-0.6575909824	2.4648602838
C	1.7076967602	2.1466342026	-0.1467400554
C	-0.3611700809	1.6751595344	-1.3841890629
H	-1.8347339246	-1.1791290986	3.4211911844
H	-1.9925412384	0.3947934012	2.613816442

H	-2.4366589536	-1.102364259	1.7551762422
C	0.9542677542	2.7075516451	0.8812998991
H	2.7897307426	2.1056934886	-0.0772763884
C	-1.1121885801	2.2704551139	-0.3400637302
H	-0.8552241213	1.3380030705	-2.2876851689
C	-0.4552723229	2.7567946284	0.7914245939
H	1.4460542872	3.080634207	1.7736126883
H	-2.1922599966	2.3382034332	-0.4199405993
H	-1.0292643797	3.1725388124	1.6133976622
Si	-0.0207493042	-1.6550280333	-0.9038604574
H	1.632578991	1.1793913834	-2.0886095548
C	-0.0417364304	-1.3543905005	-2.802083811
C	1.5213556378	-2.7253968454	-0.6066208533
C	-1.6080198245	-2.6587474408	-0.6062342814
H	-0.0138414773	-2.3321186916	-3.3033840935
H	-0.9545698518	-0.8488934618	-3.1402639022
H	0.8191090217	-0.7828209307	-3.1688734098
H	1.467931732	-3.6378512261	-1.2162409057
H	1.6139926294	-3.0151310722	0.4437773956
H	2.4351542076	-2.1916665552	-0.8959649639
H	-2.5058680893	-2.0498033953	-0.7709817241
H	-1.6521509337	-3.4981011835	-1.3135787965
H	-1.6501850376	-3.0630268013	0.4091343049

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21 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.7790386706	-0.0685160671	-0.1952535945
S	0.9814778745	-0.82475763	0.6788783111
C	1.086427543	-2.3876986414	1.6672304435
H	0.0678886227	-2.7777937852	1.7285256032
H	1.7240822228	-3.1253154389	1.1723270354
H	1.4561551758	-2.1887918331	2.6766306226
C	-1.4365802279	1.788424698	-0.5967595574
C	-0.9299015164	1.2122178582	-1.7650809959
C	-2.9110269912	1.8755135338	-0.2144792236
H	-0.7886149828	2.5029133904	-0.0850221816
C	-1.7616583193	0.4699816483	-2.797349194
H	0.0412047147	1.5562179428	-2.1225827703
C	-3.3620563242	0.7036119905	0.7074081872
H	-3.5329623356	1.9083127228	-1.1148508085
H	-3.0941857055	2.823645945	0.3062864844
C	-2.8365541755	-0.4729921106	-2.1763351461
H	-1.0758846178	-0.1321226635	-3.4079535249
H	-2.2497385844	1.1682431583	-3.4968117341
C	-2.6562148941	-0.6083986885	0.4123975108
H	-3.1432028446	0.9720205582	1.749360642
H	-4.4573452985	0.5931739038	0.6510274377
C	-2.3831831674	-1.1022920731	-0.8635296279
H	-3.7745264768	0.0716317389	-2.0283548595
H	-3.0658462136	-1.2672245864	-2.8975799108
H	-2.6216150034	-1.3093294168	1.2474062464
H	-2.0978904477	-2.1538427932	-0.9311357645
Si	3.0628340197	-0.1557834994	0.5912308008
C	4.1201956206	-1.4159394383	-0.3426946785
H	5.1572153156	-1.0651334722	-0.4245732162
H	4.141652728	-2.3883129549	0.1629246232
H	3.7358384295	-1.5728710543	-1.3566185429
C	2.9731785284	1.4757409263	-0.3494184377

H	2.5390795155	1.3350356846	-1.3451039859
H	2.3569679823	2.2078450585	0.1839452278
H	3.9761208794	1.90309468	-0.4732855862
C	3.7438545585	0.1098366138	2.3360898231
H	3.7664483246	-0.820634096	2.9149936592
H	4.7710820441	0.4948432717	2.2935829138
H	3.1348276978	0.834823919	2.8873847688

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TS$_{5A-22}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.6449949475	-0.1462385033	-0.0982196221
S	0.6908384138	-2.2717515171	-0.3603876395
C	2.4844542658	-0.0095975643	0.1292320658
C	2.2739758382	-2.9513723667	-0.9909121339
C	3.0771100118	-0.2214634572	1.3811639189
C	3.2868786241	0.3991997424	-0.9434827356
H	2.5755684058	-2.4728375347	-1.9256348673
H	3.0690688695	-2.828717414	-0.252354337
H	2.1130909947	-4.0175783784	-1.1724076907
C	4.4503672492	-0.0215926429	1.5551664867
H	2.476425294	-0.5571235889	2.2221784526
C	4.6613062605	0.5953607421	-0.7652613634
H	2.8555306348	0.5536858762	-1.9297382145
C	5.2471638368	0.389225009	0.4840968842
H	4.8961936751	-0.1928153746	2.5324151841
H	5.2709897748	0.9104094134	-1.6091682856
H	6.3144320691	0.541233745	0.6213375789
Si	-2.9932773057	-1.8790187124	0.1363580521
H	-1.8942096849	-0.8465265033	0.1909472422
C	-4.6250466057	-0.9917740073	0.5173426696
C	-3.0224226256	-2.6062836288	-1.6049643557
C	-2.6247318387	-3.1878231762	1.4450276502
H	-5.4628627276	-1.7002509665	0.49874869
H	-4.6106144765	-0.5258606442	1.5097592043
H	-4.8435569984	-0.2070975992	-0.2169331095
H	-3.2681810978	-1.8442663142	-2.3544660886
H	-3.7688364033	-3.4061931482	-1.6871761274
H	-2.0409907978	-3.0228092435	-1.8550759969
H	-3.36517823	-3.9969281306	1.4147636078
H	-1.6329849787	-3.6211325454	1.2776639033
H	-2.6408994156	-2.7601898737	2.4547561232
C	0.1982175835	1.673485273	0.7486133402
C	0.1706329979	1.7412627366	-0.6407033541
C	-0.9632482135	1.6386642955	1.7359715065
H	1.1380154349	1.975356202	1.2061493272
C	-1.0472787099	1.7701291439	-1.5425216344
H	1.0743844558	2.1261452067	-1.1141335456
C	-2.3276264653	2.1847683846	1.2504306577
H	-0.6460273264	2.2329743728	2.6027719923
H	-1.1153877503	0.621481666	2.1243819176
C	-1.5842227301	3.205607242	-1.7519236602
H	-1.8378847971	1.1157749106	-1.1713022249
H	-0.7664584771	1.3733446475	-2.5265024777
C	-2.2754303536	3.5961383631	0.7108585004
H	-2.7662651661	1.4997700774	0.5224049998
H	-3.0048962104	2.1658829836	2.11366705
C	-1.972383564	4.0032620222	-0.5282203743
H	-0.816671032	3.7801827915	-2.2902926329

H	-2.4406966778	3.1587520838	-2.44323105
H	-2.5037598283	4.3761176798	1.4376970845
H	-2.0056501492	5.0787002247	-0.7083045684

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22 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.3576443649	-0.2474136378	0.4127075902
S	-2.2860821806	0.595870894	0.9269890996
C	-1.0638716235	-1.9813956665	0.4646600625
C	-3.6962448208	-0.5624958033	1.0974857199
C	-1.0479812756	-2.7328018988	1.6481969175
C	-1.5398079092	-2.5872425955	-0.7070388134
H	-3.885338093	-1.1020497032	0.1670382622
H	-3.5245841136	-1.2846151688	1.898426417
H	-4.5703085134	0.0472609446	1.343425712
C	-1.4938442488	-4.0590697201	1.6584578127
H	-0.7023602664	-2.2841167902	2.5766676674
C	-1.985491075	-3.9134955032	-0.6954509064
H	-1.578854663	-2.0255044399	-1.6377578169
C	-1.9623857256	-4.6556793387	0.4866396213
H	-1.4752161117	-4.6236476699	2.5881513365
H	-2.3522861856	-4.3639940108	-1.615230668
H	-2.3095062712	-5.6855410546	0.4954055232
Si	-0.0617138955	3.1305186424	0.0138412176
H	0.2346329365	1.6666923775	0.3530310985
C	1.604703968	3.9878734733	-0.2584549414
C	-1.0863453042	3.1610861774	-1.5647695651
C	-0.9345365413	3.886446249	1.4987755078
H	1.432917093	5.053615082	-0.4588281525
H	2.2489676763	3.9225898399	0.6255751388
H	2.1572600977	3.5823806434	-1.1134231488
H	-0.5480918437	2.6955525352	-2.3988165582
H	-1.3179330982	4.1941903397	-1.8532789017
H	-2.0268314801	2.6215978268	-1.4167394489
H	-1.2368535645	4.9186845309	1.2810046445
H	-1.8268452649	3.3080328997	1.7552859511
H	-0.2761996062	3.9094440437	2.3751994537
C	1.5885443433	-0.8324151082	0.7356967538
C	1.327683367	-0.7953948385	-0.6297911042
C	2.4495241628	0.1077860179	1.5714761718
H	1.4337278459	-1.8009454014	1.2062103676
C	1.8676643926	0.1854901682	-1.6472738049
H	1.0249798344	-1.7429019352	-1.074491628
C	3.5984445236	0.8458910092	0.8386234587
H	2.8893154133	-0.5030340663	2.3700219608
H	1.8311276538	0.855108378	2.0879482384
C	3.2398360121	-0.2698076165	-2.1992099076
H	1.938418695	1.1949046203	-1.243776431
H	1.1713752596	0.2435908032	-2.4944599396
C	4.5150573636	-0.0568217523	0.044192912
H	3.1905806123	1.6365112345	0.2065213206
H	4.1909854523	1.3608323311	1.6056279991
C	4.3582721412	-0.5040453627	-1.2084442649
H	3.0902729651	-1.2072190811	-2.7538724537
H	3.5710152368	0.4584110864	-2.9569339438
H	5.4090514041	-0.3889214438	0.5725704938
H	5.1525965903	-1.1414925412	-1.599319032

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$TS_{22\text{-}23A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.4200963365	0.3495420474	-0.2077221489
S	-3.2293312869	0.1976298946	-1.2941408451
C	-1.3064033632	-1.4146098953	0.3017077006
C	-4.2028008832	-1.3183735682	-0.9493559758
C	-1.4329429533	-1.7539290559	1.6619721594
C	-0.8538897592	-2.411363004	-0.5840406534
H	-3.697175749	-2.2137372669	-1.315790575
H	-4.4072709734	-1.4335264673	0.1175586519
H	-5.1510004065	-1.1974232647	-1.4832135091
C	-1.0767136612	-3.0248687669	2.1264654507
H	-1.8199884449	-1.0300947905	2.3767509739
C	-0.4985328082	-3.6817385296	-0.1226672084
H	-0.7888880461	-2.197098581	-1.6484335112
C	-0.6054990698	-3.9907845876	1.2363464839
H	-1.1763857353	-3.2612882023	3.1836536454
H	-0.1477251196	-4.434613266	-0.8253358675
H	-0.3360393323	-4.9808065355	1.5954968751
Si	-1.1652507519	2.8780693151	0.3814681855
H	-1.0947336291	1.8898114848	-0.8081617554
C	0.3122434077	3.9859614014	0.0105800843
C	-2.8157539236	3.7663176924	0.2853755194
C	-0.9255096632	2.0135169176	2.0541715206
H	0.4094242097	4.7739495764	0.7677407307
H	1.2378577065	3.3997600156	0.0086510731
H	0.2160031063	4.4715632875	-0.9670645214
H	-2.9286866696	4.2795726729	-0.6760492256
H	-2.9027064033	4.5164465659	1.0812063933
H	-3.6419715782	3.0549437754	0.3814652297
H	-0.5074478221	2.7358046453	2.7686601831
H	-1.8764332543	1.6551943122	2.4606741872
H	-0.2324504095	1.1640600954	2.0228448961
C	2.82893258	0.9290363654	0.7888705168
C	2.0891752194	0.3174115782	-0.1456380615
C	4.2941650306	1.2935500106	0.7997276198
H	2.311394716	1.2099642541	1.7079966867
C	2.4955405561	-0.2194365966	-1.4999690168
H	1.044420118	0.1223305243	0.110486187
C	5.2054019483	0.6597995033	-0.273619704
H	4.6904152104	1.0299685	1.7914746181
H	4.3860491546	2.3901559201	0.7392381106
C	3.1439044471	-1.6194890827	-1.4361872462
H	3.1510582462	0.4769116406	-2.0283758882
H	1.5934446599	-0.3053196751	-2.1183059173
C	5.2857989696	-0.8505349942	-0.1950859702
H	4.898616518	0.9951897681	-1.2674457154
H	6.2135563521	1.0667293574	-0.1257606032
C	4.4355667369	-1.7692648023	-0.6706133535
H	2.412922901	-2.3147658816	-0.9990550515
H	3.3013593684	-1.9787515535	-2.4660521126
H	6.1506541314	-1.2299024079	0.3500680664
H	4.7012427393	-2.8115903463	-0.4860733121

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23A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.2476530345	0.4814457575	-0.2251873979

S	-1.3602548472	-0.1420206495	-2.260412018
C	-1.9556529234	-1.1143502283	0.4512083991
C	-2.0552924116	-1.815975266	-2.5393230449
C	-3.3221950792	-1.2164982985	0.7608548287
C	-1.1186066426	-2.186118672	0.804083451
H	-1.4408880375	-2.5922975498	-2.0793051102
H	-3.0768153488	-1.8971667649	-2.161791641
H	-2.0607167186	-1.9589171308	-3.624630974
C	-3.8331203715	-2.344352747	1.411235048
H	-4.0058254854	-0.4150558827	0.4867055893
C	-1.6259778366	-3.314108137	1.4574180007
H	-0.058529159	-2.1528520036	0.5605313719
C	-2.9856320807	-3.3967082647	1.7636314008
H	-4.8953985188	-2.4011888229	1.6392892439
H	-0.9575193822	-4.1304661794	1.722503256
H	-3.3823394326	-4.2752796836	2.2660858765
Si	-1.014057663	2.8379696706	0.2068257599
H	-0.5573442704	1.8788277601	-0.9079400847
C	0.4991810521	3.9248359607	0.4697466661
C	-2.5388741881	3.7880139055	-0.3374554769
C	-1.294127728	1.7517969024	1.747207905
H	0.3300068711	4.6485075789	1.2764462748
H	1.3668639039	3.3130829297	0.7421063828
H	0.7559232088	4.4865624119	-0.4351271018
H	-2.3597656655	4.2874468743	-1.2960511325
H	-2.8036735788	4.5562149408	0.3994037612
H	-3.398971196	3.1225112939	-0.4631403617
H	-0.5538651815	2.0474715432	2.4998239684
H	-2.2966954892	1.876791503	2.1652169732
H	-1.1423747654	0.6532402482	1.6525081865

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23B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.3409217449	0.3120970901	0.9468155713
S	2.2199510218	-0.1381082267	1.7404374693
H	-1.1509506941	0.8798778593	0.8868962777
Si	-1.1480824851	2.0574912756	-0.1462891846
C	0.4256814684	2.4636663502	-1.1136768537
H	0.7438320498	1.6329588302	-1.75073639
H	0.2134203918	3.3200388373	-1.7697153267
C	-2.5098564257	1.5169455675	-1.3243102203
H	-3.449626542	1.3170596097	-0.7981390188
H	-2.7024536588	2.2867245008	-2.0814489182
C	-1.6033778863	3.5164926713	0.9575818189
H	-1.7955919429	4.411953024	0.3536002688
H	-2.5009950614	3.3136902069	1.5520425813
H	1.2633009651	2.7441583495	-0.4671739981
H	-0.7877613686	3.7547057502	1.6504518654
H	-2.21138204	0.5977511774	-1.8401724126
C	-0.1635530428	-1.2001077752	0.0124177074
C	-1.140989874	-2.0567199713	0.5391046882
C	0.3806795036	-1.4932874707	-1.244746496
C	-1.5733078222	-3.1723083248	-0.1833456061
H	-1.5732683036	-1.862495994	1.5180075628
C	-0.0602816357	-2.6051592118	-1.9724909762
H	1.1615635527	-0.8656966176	-1.6701436501
C	-1.0378971292	-3.4482525641	-1.4437583679
H	-2.3311086746	-3.8266098064	0.2418498736

H	0.3709573723	-2.8138711513	-2.9490787568
H	-1.3756024381	-4.3157272123	-2.0046962756
C	3.463816421	-0.0157429538	0.391239186
H	4.447009012	-0.2195131609	0.8233563299
H	3.2591271961	-0.7717102523	-0.3726887859
H	3.4801573257	0.9739975933	-0.0732739632

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CP1 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.52534	-0.92208	-0.10411
C	1.45937	-1.29247	0.67903
C	1.51081	-1.1342	-0.68642
C	1.9365	0.07601	-1.49438
C	3.46454	0.1905	-1.67144
C	4.30728	0.40695	-0.43978
C	3.96339	0.72993	0.81339
C	2.59025	0.9564	1.41342
C	1.86658	-0.3515	1.79527
H	1.29571	-2.31447	1.02508
H	1.42574	-2.0542	-1.26999
H	1.52973	0.99691	-1.07601
H	1.49158	-0.01479	-2.49243
H	3.83074	-0.71546	-2.17715
H	3.66335	1.00961	-2.38002
H	5.37486	0.28295	-0.62963
H	4.78398	0.8175	1.5255
H	1.94921	1.56615	0.7726
H	2.71387	1.53491	2.33684
H	2.52854	-0.93134	2.45454
H	0.99031	-0.11232	2.41471
S	-2.00532	-2.46807	-0.36724
C	-1.37129	0.79475	-0.08376
C	-2.04342	1.29071	-1.21608
C	-1.30998	1.62863	1.04831
C	-2.60671	2.56939	-1.22823
H	-2.14212	0.6678	-2.10267
C	-1.87616	2.90797	1.04646
H	-0.82288	1.28564	1.9607
C	-2.52018	3.38447	-0.09658
H	-3.11831	2.92782	-2.11914
H	-1.81388	3.53053	1.93716
H	-2.95989	4.37879	-0.1024
C	-3.26177	-2.28637	0.9613
H	-3.65986	-1.26888	0.97413
H	-4.07818	-2.98309	0.75211
H	-2.84303	-2.52363	1.9438

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5B^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.6496375895	-0.8514718261	0.4368506582
C	1.4909348508	-1.3001084073	0.8327838443
C	1.3887562063	-1.1547795714	-0.5207803372
C	1.7079958528	0.0435124448	-1.38633393
C	3.2110887634	0.1530287596	-1.7171168884
C	4.168363167	0.3959970952	-0.5767525624
C	3.946907372	0.7412747307	0.6981171264
C	2.6368534115	0.984166149	1.4192365892

C	1.9454070368	-0.3123664794	1.8888442068
H	1.3551608574	-2.3133470778	1.2117870948
H	1.1994962901	-2.0742886137	-1.0751199003
H	1.3419305049	0.9695092459	-0.9445496564
H	1.1611317511	-0.0685634596	-2.3294325788
H	3.5289201921	-0.7644098959	-2.2343630525
H	3.3385127915	0.955358248	-2.4604662265
H	5.212883006	0.270494338	-0.8661110706
H	4.8312604117	0.8420023771	1.327595198
H	1.9409966627	1.5847659669	0.82953733
H	2.845189961	1.5775685756	2.3175830594
H	2.6368245651	-0.8631418505	2.5419899992
H	1.0966924939	-0.0508866539	2.5412637556
S	-1.5625680099	-2.7403018976	-0.172985647
C	-1.294355772	0.9502204721	0.1701191597
C	-1.9263998211	1.3381966616	-1.0277553593
C	-1.2131824374	1.9266709233	1.184644071
C	-2.4471096282	2.6220773692	-1.2081735598
H	-2.0219214644	0.6199649351	-1.840740646
C	-1.7273878734	3.2168423595	1.0157335267
H	-0.7404598272	1.6904231601	2.1389374139
C	-2.3465919916	3.5677134235	-0.1846859897
H	-2.9306778629	2.8868531365	-2.1461848168
H	-1.6469926213	3.9449417337	1.8203189111
H	-2.7488409233	4.5686327387	-0.3213914457
C	-3.2409804082	-2.6972210883	0.5810435353
H	-3.7517895167	-1.7613427037	0.336924626
H	-3.8207657957	-3.5267936721	0.1681608881
H	-3.1976526058	-2.8097606466	1.6683576735

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5A^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	0.9916075206	-0.6850422567	0.7271556838
S	0.3854087235	0.2519344537	2.5942299108
C	2.7490580349	-0.5111128956	-0.0546813992
C	2.9796227363	0.0560008605	-1.3233191253
C	3.8808481523	-0.9762909211	0.6428328984
C	4.2603030523	0.134830735	-1.8795027863
H	2.1466370192	0.4631507132	-1.8987158849
C	5.1670711183	-0.9065397265	0.0981684751
H	3.7635295024	-1.4000286549	1.6397889122
C	5.3596871066	-0.3509976689	-1.1682181499
H	4.4020791887	0.5803818072	-2.8621753005
H	6.0187927213	-1.2801386532	0.6630034099
H	6.3581100384	-0.2909765289	-1.594824275
C	1.4088703206	1.7787548435	2.6997366504
H	0.9736220571	2.5723369687	2.0860313641
H	1.4216712918	2.1070452394	3.7421437293
H	2.4321956058	1.5884011562	2.3691263957
S	-0.5249325284	-1.0036572355	-1.1010195805
C	-2.0327445517	-1.7434638238	-0.4575402091
C	0.2045048653	-2.4043670934	-2.0357206438
C	-3.1819632587	-1.7537297414	-1.2570208426
C	-2.0700276445	-2.2701061816	0.8381070136
H	0.2827533165	-3.2920249114	-1.404377868
H	-0.4103549343	-2.6179684381	-2.9122711447
H	1.2022274845	-2.0831901346	-2.3439591284
C	-4.3609578827	-2.3134129582	-0.763478396

H	-3.1529782015	-1.3220359894	-2.2531075236
C	-3.2546334861	-2.8209481596	1.3278592611
H	-1.1825889351	-2.2403271025	1.4633948219
C	-4.3980678981	-2.8465552328	0.5271777838
H	-5.2524112213	-2.323605131	-1.3842414856
H	-3.2818446779	-3.2231060173	2.3362723065
H	-5.3198246361	-3.2742993208	0.9111981269

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$TS^3_{5A\text{-}18A}$ B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	0.9215694375	0.1913910148	0.3810879908
S	0.4164359526	1.8435897556	1.6981752536
C	2.7652927823	-0.0393474646	-0.1763987621
C	3.1315464633	-0.0991780496	-1.5349114579
C	3.8028025967	-0.183509108	0.7631335617
C	4.4572804769	-0.2963211687	-1.9369485548
H	2.3732723456	0.0155111857	-2.3108219666
C	5.1319425362	-0.3850706904	0.3750271057
H	3.5773116297	-0.1389069432	1.8287749925
C	5.4636241502	-0.4414294133	-0.9798425594
H	4.7043923858	-0.3336821975	-2.9961626575
H	5.9081856922	-0.4952790768	1.1297633673
H	6.4954071699	-0.5942283759	-1.2870760474
C	1.9082161553	2.9107665807	1.858781945
H	1.7863244197	3.7990083375	1.233183085
H	2.0014341	3.2216183297	2.9023719693
H	2.8105490176	2.3781964712	1.5526565881
H	-1.8123258848	0.8156566564	-1.4406165344
Si	-2.7164225804	2.0054563241	-1.3255446782
C	-3.4139887611	2.0623742892	0.4297849888
H	-4.1201137872	2.8938788978	0.5481652968
H	-3.9428947123	1.1362299623	0.6845819626
C	-1.698817563	3.55533977	-1.6939334037
H	-0.884789807	3.6547062024	-0.9666873809
H	-2.3155065685	4.4607128883	-1.6331916747
C	-4.1043960725	1.7899875887	-2.5985328135
H	-4.8016673084	2.636648105	-2.5705193
H	-3.7055379502	1.7231605088	-3.6178228746
H	-2.6040098653	2.2033261548	1.1548790155
H	-1.2566814464	3.5205392237	-2.6968319222
H	-4.6831980379	0.8783789587	-2.4073233293
S	-0.1804342832	-1.7034774677	-0.7649687173
C	-1.6239179852	-2.1137367062	0.2278013612
C	0.9530534788	-3.0953292161	-0.3776236925
C	-2.6127817619	-2.946614442	-0.309319877
C	-1.7725847862	-1.5794066803	1.5128738029
H	1.0565260937	-3.2216739756	0.7020020144
H	0.5730672761	-4.012253359	-0.8324268909
H	1.9205319331	-2.8291369258	-0.8090388853
C	-3.7407637485	-3.2578094369	0.4512144455
H	-2.500918593	-3.34083452	-1.314952869
C	-2.9059661997	-1.8907104586	2.2651611263
H	-1.0117678931	-0.9177159724	1.9185276913
C	-3.8877756095	-2.7315496441	1.7369508152
H	-4.5076653848	-3.9054752934	0.0356822927
H	-3.0198559961	-1.4710286229	3.2603536377
H	-4.7699125069	-2.9715199961	2.3238415393

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18A^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-1.3097295685	-0.3394797148	-0.8321805933
S	-1.2411565126	-2.3498902754	-1.6740790478
C	-2.2735966382	1.232036892	-0.2800116378
C	-1.9420600749	-2.1934028738	-3.3710896783
C	-1.7327679403	2.1456591535	0.6468760645
C	-3.5227815667	1.5674215166	-0.8376328618
H	-2.9856597991	-1.867218877	-3.3343253194
H	-1.3685080671	-1.4937028638	-3.9852790156
H	-1.9060385298	-3.1794896746	-3.840164628
C	-2.3875528358	3.3341674556	0.9864832031
H	-0.7705503208	1.9387161439	1.1154462369
C	-4.1915325372	2.7475055737	-0.5023948518
H	-3.9990828826	0.8913255611	-1.5475583209
C	-3.6228971755	3.6369422687	0.4123219258
H	-1.9360843769	4.0197290404	1.7006253303
H	-5.1566285983	2.9728613959	-0.9511523508
H	-4.1404043634	4.5556344934	0.677615301
Si	-0.7612160916	-1.4972274341	2.0371074402
H	-0.4472711662	-0.7461622185	0.733957316
C	-2.6271177136	-1.6850362744	2.1751295347
C	0.1172473355	-3.1522609549	1.8717302413
C	-0.0535126708	-0.4084947673	3.4038312652
H	-2.8899996344	-2.144121995	3.1366373169
H	-3.130054944	-0.7143581898	2.112243429
H	-3.0186421352	-2.3260807533	1.3778151507
H	-0.2378429202	-3.6817476676	0.9806072817
H	-0.0743905206	-3.7875406817	2.7454937838
H	1.2020359808	-3.0266876257	1.7803242723
H	-0.2017886931	-0.8766150307	4.3850728272
H	1.0221410561	-0.2445686173	3.273076548
H	-0.547665095	0.569159995	3.4225998369

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TS^3$_{18A\text{-}18B}$ B3LYP/BSI Optimized geometry (charge = 0, triplet)*

Ni	-0.295539	-0.082819	0.641722
S	-0.147465	1.205659	2.436052
C	-1.734798	-1.246951	0.056816
C	0.065662	0.05229	3.853307
C	-1.749297	-1.955581	-1.160662
C	-2.854134	-1.426224	0.893312
H	0.185212	0.647186	4.762738
H	-0.815434	-0.585306	3.974415
H	0.949843	-0.584348	3.741298
C	-2.807812	-2.796024	-1.524202
H	-0.919167	-1.857225	-1.861681
C	-3.917084	-2.266641	0.54683
H	-2.906018	-0.891506	1.841026
C	-3.896895	-2.956893	-0.666574
H	-2.780491	-3.325047	-2.474906
H	-4.762295	-2.380718	1.222648
H	-4.721309	-3.61022	-0.94195
Si	-1.465449	2.369781	-1.092347
H	-0.433599	1.423067	-0.47613
C	-2.966171	2.440232	0.035456
C	-0.58268	4.033245	-1.214043

C	-1.880677	1.647124	-2.782781
H	-3.704544	3.152042	-0.355183
H	-3.444737	1.458227	0.110528
H	-2.682646	2.755563	1.045233
H	-0.279696	4.386722	-0.222079
H	-1.241975	4.792234	-1.653506
H	0.315292	3.969781	-1.839397
H	-2.635728	2.259044	-3.291946
H	-0.999658	1.59915	-3.433634
H	-2.283892	0.634008	-2.676796
C	2.233122	-1.267395	0.827628
C	1.735239	-1.318432	-0.425947
C	3.241006	-0.335168	1.450459
H	1.869695	-2.036023	1.513011
C	2.090112	-0.453029	-1.617598
H	1.076734	-2.157841	-0.647616
C	4.141823	0.490258	0.506363
H	3.881921	-0.94823	2.099902
H	2.705487	0.353236	2.121469
C	3.364165	-0.924284	-2.352636
H	2.186767	0.597628	-1.336238
H	1.261156	-0.495183	-2.335326
C	4.994116	-0.348751	-0.422574
H	3.539012	1.216971	-0.04387
H	4.806915	1.088577	1.140554
C	4.664394	-0.924455	-1.58573
H	3.193017	-1.94646	-2.72094
H	3.486173	-0.312223	-3.260437
H	6.012656	-0.519793	-0.073246
H	5.451564	-1.491756	-2.08469

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$TS^3_{18B\text{-}23A}$ B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.2829335131	-0.0699945751	0.7375288448
S	0.5013259146	0.8447750537	2.5681313294
C	-1.6973019416	-1.2235248316	0.1083040852
C	1.1225923408	-0.5304933589	3.623930493
C	-1.8963949705	-1.501127835	-1.2591708756
C	-2.5695831262	-1.8556647725	1.0147512357
H	1.5586521562	-0.0884337408	4.5231837382
H	0.304266153	-1.1906903849	3.9258791953
H	1.8919385221	-1.1198466119	3.1174130825
C	-2.900677794	-2.3703424093	-1.6987272438
H	-1.2523707453	-1.0365379251	-2.0048458593
C	-3.5774545927	-2.7259274783	0.5877615773
H	-2.4719496195	-1.6646277672	2.0830509154
C	-3.745320112	-2.9863996987	-0.7736012958
H	-3.0237768137	-2.5652139286	-2.7622001241
H	-4.2332753557	-3.1979263975	1.3163355655
H	-4.52894028	-3.6606894507	-1.1105476427
Si	-1.7316212246	2.5669715681	-0.1950681173
H	-0.6153541907	1.5215627135	-0.0868123474
C	-2.9802593692	2.2447642668	1.1724906018
C	-0.8512292743	4.2196939076	0.0154071904
C	-2.4710716652	2.3332452033	-1.9108760744
H	-3.7928061383	2.9808997779	1.1245655028
H	-3.4201374745	1.2463632476	1.0779566376
H	-2.5110728401	2.3189462787	2.1595664099

H	-0.3511176055	4.2688871523	0.9891005392
H	-1.5637371274	5.0521823009	-0.0400988553
H	-0.0944037763	4.375394534	-0.7618104097
H	-3.2911875294	3.0421530242	-2.0800848429
H	-1.7253393258	2.4922056179	-2.6981449289
H	-2.8722124039	1.3198524633	-2.0206966825
C	1.7275645429	-1.0532094186	-2.0754839195
C	1.9151151528	0.2757421753	-2.0776093399
C	2.0781237981	-2.1084181504	-1.0556923881
H	1.2361139121	-1.4673865976	-2.9574800299
C	2.573447639	1.1681533889	-1.0437843759
H	1.5751047546	0.7987318952	-2.9723771177
C	2.9493155983	-1.6861090422	0.1450286831
H	2.5820675363	-2.9299526986	-1.5859238685
H	1.1390921762	-2.5471188307	-0.6817509663
C	4.1155039466	1.146333162	-1.0710060084
H	2.2153567043	0.9551458498	-0.0331944331
H	2.2622307734	2.201261125	-1.2434121168
C	4.3618568392	-1.2951529471	-0.2331889713
H	2.4418108942	-0.8940475804	0.7048495911
H	3.0023572699	-2.5428276283	0.8284137902
C	4.8217949894	-0.1434772941	-0.7374146644
H	4.4522764366	1.4613569092	-2.0703133411
H	4.4826815501	1.9282167744	-0.3873896442
H	5.0982026118	-2.088057173	-0.0986174523
H	5.892447597	-0.104701863	-0.9461200713

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23A^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.3758198778	-0.0639787782	0.7794734628
S	0.6039835916	1.0857053375	2.3522439883
C	-1.7268083082	-1.2934285174	0.1737317819
C	1.205366448	-0.1617585497	3.5678436324
C	-2.1255465832	-1.349756013	-1.176892518
C	-2.3140485331	-2.2339104463	1.042346414
H	1.7248118617	0.3728721713	4.3666142769
H	0.3692159244	-0.7124106637	4.0088389064
H	1.9019826068	-0.8709189686	3.1122302268
C	-3.0420313178	-2.2988352019	-1.6415676069
H	-1.7087187647	-0.6447340058	-1.8962234999
C	-3.2360881355	-3.1829580668	0.5935932314
H	-2.0576504498	-2.2281061383	2.1016813692
C	-3.6022507148	-3.218436206	-0.7539244353
H	-3.320868493	-2.3173230198	-2.6931026863
H	-3.6715573067	-3.8926967363	1.2937477047
H	-4.3207355632	-3.9539731179	-1.1074138589
Si	-1.6896351232	2.5577767274	-0.3495208316
H	-0.7283274807	1.3594522624	-0.3214757919
C	-3.0914729007	2.2184737087	0.8569742222
C	-0.6440223777	4.03562675	0.1612497995
C	-2.2937088338	2.6500298126	-2.1329925389
H	-3.8409828787	3.0179903785	0.7987810665
H	-3.5882779917	1.2688242962	0.6323251671
H	-2.7229042434	2.176941028	1.8876837444
H	-0.2061847228	3.8652297722	1.1511018388
H	-1.2509048144	4.9484196334	0.208741864
H	0.1751629008	4.2143175528	-0.5443700087
H	-2.9713043531	3.5026408677	-2.2666660974

H	-1.4614326729	2.7738022826	-2.835127127
H	-2.8411978925	1.7422608484	-2.4096586965

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23B^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.0036978515	0.9376419274	-0.0524285339
S	-0.9802826285	2.8458211869	0.3928568042
C	1.6589149046	-0.0355355748	-0.068975032
C	-0.8696075853	3.8179002282	-1.1699932086
C	1.9005369045	-1.09859235	-0.9593575351
C	2.7005381922	0.2965157949	0.8165402859
H	0.1726658678	4.0092439071	-1.4399270313
H	-1.3692824591	3.3099093123	-2.0001611224
H	-1.3641362575	4.7773673272	-1.0022347703
C	3.1115550855	-1.7996556183	-0.9648077338
H	1.1322966398	-1.397442817	-1.6728206547
C	3.9128905172	-0.3993955944	0.8259993346
H	2.5733018001	1.119421397	1.519307433
C	4.1219693213	-1.4519005272	-0.0675879194
H	3.2647184459	-2.6149382643	-1.6689547697
H	4.6953912226	-0.1186027555	1.5277563136
H	5.0642547544	-1.9944230177	-0.065448546
Si	-2.0040014991	-1.4093960184	0.0516850274
H	-1.1211290988	-0.5145298122	-0.8092622002
C	-1.5994769187	-1.0200162297	1.8558227787
C	-3.7826591222	-0.9538014817	-0.3651099231
C	-1.5522960217	-3.1844377378	-0.386139449
H	-2.1604269092	-1.6935591816	2.5159838164
H	-0.5349315907	-1.1618692006	2.0765401038
H	-1.8811695618	0.0039162311	2.1304922833
H	-3.9659844313	0.1070233454	-0.1602491374
H	-4.4905289135	-1.538905428	0.2347713521
H	-4.0093016301	-1.138686164	-1.421319847
H	-2.1195106857	-3.8961182977	0.2262592685
H	-1.7651591749	-3.4057986991	-1.4381645611
H	-0.4857043164	-3.3645938875	-0.2118328262

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CP2 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.22692	0.69893	-0.11253
S	-0.82781	2.69817	0.43687
C	1.50534	-0.08837	-0.07766
C	-0.55159	3.7548	-1.04732
C	1.84066	-1.23309	-0.82162
C	2.52438	0.50365	0.68938
H	0.51709	3.83463	-1.26518
H	-1.07012	3.36872	-1.92946
H	-0.93671	4.75377	-0.82604
C	3.13357	-1.76845	-0.80143
H	1.08997	-1.72454	-1.43953
C	3.81772	-0.02557	0.71808
H	2.3092	1.3941	1.27593
C	4.12583	-1.16471	-0.02896
H	3.36278	-2.65577	-1.38813
H	4.58687	0.4537	1.3201
H	5.13143	-1.57698	-0.0101
Si	-2.0178	-1.50232	0.02677

H	-1.01232	-0.72554	-0.83673
C	-1.65603	-1.16715	1.8491
C	-3.71308	-0.87125	-0.48896
C	-1.72167	-3.30907	-0.41304
H	-2.29406	-1.80667	2.47317
H	-0.61449	-1.39199	2.10336
H	-1.86379	-0.12966	2.13525
H	-3.82903	0.19214	-0.2516
H	-4.50893	-1.42034	0.0292
H	-3.86869	-0.99511	-1.56663
H	-2.4299	-3.95916	0.1157
H	-1.84359	-3.48822	-1.48718
H	-0.70858	-3.61609	-0.1316

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$TS_{23B\text{-}18B}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.1200828918	-0.9582522993	0.3225787428
S	0.5224722112	-0.4725102845	1.5502396719
H	-2.3727201959	-0.8511105045	-0.4274208825
Si	-2.2718867676	0.9212718373	-0.3489377008
C	-0.9204498064	1.9129667239	-1.2283401258
H	-0.5550556985	1.3894855177	-2.1193127587
H	-1.3403224315	2.8718921222	-1.5618939663
C	-3.7611195801	0.860849226	-1.5248640487
H	-4.6030432016	0.3046204349	-1.0970571942
H	-4.108728716	1.8797667747	-1.7412661451
C	-2.825220519	1.689226954	1.2866523723
H	-3.2975512491	2.6616311168	1.0915017796
H	-3.5674214464	1.0580298321	1.7886769326
H	-0.0676561019	2.1185456108	-0.5751491709
H	-1.985155476	1.8389346338	1.9708399553
H	-3.5024000227	0.3883919598	-2.4797702622
C	-1.9421484791	-2.4859265441	-0.3923488171
C	-2.7242343616	-3.2959497621	0.4442803248
C	-1.5569532874	-2.9713959298	-1.6504498888
C	-3.0585753567	-4.5946427035	0.0528257508
H	-3.0654672613	-2.9254412749	1.4079016399
C	-1.8929651164	-4.2714292464	-2.0370578339
H	-0.9859969552	-2.3439864781	-2.3313718686
C	-2.6416239064	-5.086963793	-1.1859724372
H	-3.648293951	-5.2210586745	0.7177402374
H	-1.5722495718	-4.6442085577	-3.0068751793
H	-2.9088221965	-6.0951118546	-1.4909754905
C	1.9875511306	-0.2450892278	0.4548240226
H	2.8595998621	-0.0607582037	1.0869992837
H	2.1756073611	-1.135077397	-0.1506548337
H	1.8505748931	0.6146222716	-0.2075497493

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18B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.2978383768	-0.1424930561	0.3074943504
S	0.0727435804	-1.3294043562	2.0249642798
C	0.4432708109	1.6506947725	-0.6146298728
C	-1.6965210944	-1.1258570235	2.5054944914
C	1.3543145756	2.4810317088	0.0642109369
C	-0.7934318372	2.1658326764	-1.0389158373
H	-1.820113648	-1.5955372158	3.4854140584

H	-1.9848822319	-0.0747048661	2.5848164687
H	-2.3585807553	-1.6294874873	1.7959103528
C	0.9903385976	3.7862681037	0.3885487885
H	2.3323689934	2.1011713474	0.3444459837
C	-1.1490207423	3.4735017657	-0.7098298285
H	-1.4696389019	1.5420460063	-1.6154184756
C	-0.2612218201	4.2806738	0.0067748826
H	1.6837643517	4.4224298255	0.931254737
H	-2.1137766613	3.866637437	-1.0180457441
H	-0.5385656365	5.3011145805	0.2564364066
Si	0.0052101924	-1.9109774385	-0.9931115876
H	0.8245461292	0.6987364411	-1.0911734121
C	0.0631241863	-1.2740680554	-2.8016976715
C	1.3893010746	-3.1999158983	-0.8233672315
C	-1.685631943	-2.7613713001	-0.8209631121
H	-0.0718527301	-2.1231942221	-3.4864404283
H	-0.7348426647	-0.5531618093	-3.0189901104
H	1.019188001	-0.7993507956	-3.0536991967
H	1.2587769506	-3.9963762837	-1.5687482383
H	1.3813898667	-3.652118634	0.1731057134
H	2.3785483485	-2.7553927302	-0.9852835452
H	-2.5130328959	-2.0453555008	-0.896693561
H	-1.8143189992	-3.4955572483	-1.6280027429
H	-1.777383474	-3.2886475435	0.1339041456

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$TS_{23B\text{-}24}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.1118177827	0.379967316	-0.9572209626
S	-2.1762815943	-1.5447101962	-0.9843980675
C	0.0574509849	1.7628259985	-0.717072862
C	0.1934384004	3.1309072035	-0.9789162274
C	1.0821375921	1.1111331404	-0.0095380538
C	1.3163668689	3.828653976	-0.5260689535
H	-0.5773775029	3.6588111763	-1.5339585423
C	2.2072958643	1.8039772353	0.4490859804
H	1.0211024781	0.0353451773	0.2002024564
C	2.3223448896	3.1702923871	0.1884809915
H	1.4087012485	4.8928521427	-0.7315611181
H	2.9873910654	1.2824299184	0.9989687237
H	3.1934196374	3.7196718313	0.5360702239
C	-1.3198914118	-2.5792089166	0.2867525577
H	-0.9067981646	-1.9823667327	1.1035417966
H	-2.0327726749	-3.2959761624	0.6987221887
H	-0.5079073775	-3.1202026784	-0.2043655019
H	-1.7018757254	1.2015214494	-1.959395244
Si	-3.2500617371	0.2706759987	0.2079416689
C	-4.7521392087	0.433065704	-0.9251122867
H	-5.1859075146	-0.5384884072	-1.1798317361
H	-5.5199609556	1.0365484861	-0.4239069089
C	-3.6122161308	-0.7138475375	1.7898431185
H	-4.0210676768	-1.7112056876	1.5999377204
H	-4.3389201334	-0.1569970641	2.3955298891
C	-2.8696492593	2.0175561871	0.8845971832
H	-3.7278124409	2.3221480207	1.5034134406
H	-1.9750425036	2.0481274917	1.513757959
H	-4.4877711503	0.9433973364	-1.8575868094
H	-2.7104381019	-0.8257209346	2.404487379
H	-2.7372039824	2.7513041405	0.0861049967

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24 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.6552316524	0.1351697737	0.4953815862
S	-0.5763092422	-1.7147581434	0.7937552269
C	1.9072846027	1.3063310622	-0.1400902787
C	1.8385107081	2.649830477	-0.5425797777
C	3.1073679898	0.6135005031	-0.3947419735
C	2.9145226438	3.2698584567	-1.1836909965
H	0.934734587	3.223150777	-0.3502530753
C	4.1875282854	1.2254973529	-1.0381369829
H	3.2160797671	-0.4294905984	-0.086603586
C	4.0923859047	2.5604645805	-1.4353332464
H	2.8350793644	4.311679667	-1.488820226
H	5.101707048	0.6646883554	-1.2237124093
H	4.9294453592	3.0457648962	-1.931667473
C	-0.43931153	-2.4653605965	2.4725471111
H	-0.6139181923	-1.7215762154	3.2522958413
H	-1.1506857136	-3.2888229823	2.5657062743
H	0.5750471337	-2.8573750049	2.5670488118
H	0.1020156893	1.2126562133	1.2618926103
Si	-2.6534950136	-0.963618436	0.7046183407
C	-2.7468475609	-0.0715206555	-0.9479909543
H	-2.5369958614	-0.7435157047	-1.787473563
H	-3.7542610289	0.339502794	-1.0918251986
C	-3.8128424626	-2.451361746	0.7646052081
H	-3.6212351736	-3.1394609521	-0.0658082976
H	-4.8548268903	-2.1143204915	0.6900136746
C	-2.9658254003	0.2057577656	2.1454176671
H	-3.9771521446	0.6262519801	2.071068013
H	-2.8923082952	-0.2969996243	3.1165218636
H	-2.0324134959	0.7571140333	-0.987202306
H	-3.7179927794	-3.0133702693	1.700802231
H	-2.2473589509	1.0312047325	2.1316948848

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5C^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.251556754	0.5381726996	0.4665322916
S	0.37169643	-0.0049472007	2.4770704022
C	-0.3018710969	1.2541862272	3.632255701
H	-1.3658607839	1.0793280056	3.8159734873
H	0.2362018175	1.166695947	4.5796235861
H	-0.167142477	2.2596770501	3.228055466
C	-3.984351834	-2.4319232491	-1.4608661052
C	-3.9959364128	-1.3674335319	-2.2733296278
C	-3.4950136749	-2.5855766396	-0.0414939725
H	-4.3990266261	-3.3545293431	-1.8697724781
C	-3.500054291	0.0418000751	-2.0223329712
H	-4.3978419087	-1.5310806399	-3.2734645939
C	-2.610030327	-1.4653843582	0.5443068614
H	-2.9442033969	-3.5355275885	0.0230327696
H	-4.3636935085	-2.7177640281	0.6223141288
C	-1.9806044635	0.2150440817	-2.2308987482
H	-3.7907604501	0.4043298438	-1.0329849054
H	-3.9960714194	0.7127108952	-2.7338826729
C	-1.3061727898	-1.3015564507	-0.2052804349
H	-3.1685994215	-0.5289532115	0.5902600896

H	-2.3684573575	-1.7219774231	1.5811287467
C	-1.0506972406	-0.5774618271	-1.3361784694
H	-1.7387315495	-0.0890040487	-3.2592343131
H	-1.724557419	1.2804246794	-2.1715216469
H	-0.5153154127	-1.9798498058	0.1221105776
H	-0.0640916705	-0.7335277279	-1.7801658274
C	-0.4749872328	2.4402092928	0.230988278
C	0.6526974194	3.2797750664	0.325904345
C	-1.7088776301	3.0650259723	-0.0300399239
C	0.5616543532	4.6623800999	0.1362283808
H	1.6264172569	2.8520135837	0.5607456694
C	-1.8150709322	4.4470670648	-0.2126825532
H	-2.6207463782	2.4700680006	-0.0881713304
C	-0.6752493807	5.2504542388	-0.13479091
H	1.4539646455	5.2808057209	0.2080535502
H	-2.785336341	4.8974327813	-0.4121542896
H	-0.7521947417	6.3257687478	-0.2762775573

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$TS^{3}_{5C\text{-}9A}$ B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.2790890104	0.2497842637	0.5971808853
S	0.1786475433	-0.1473558393	2.7005879311
C	-0.3507103986	1.3119962025	3.6824771809
H	-1.4301235152	1.2862830707	3.8562339832
H	0.1603075153	1.27497251	4.6480833359
H	-0.0918596872	2.2394352903	3.1675589484
S	2.055339713	-3.0225121941	0.2235166338
C	2.9433587154	-1.6335484055	-0.4676633091
C	2.5380118614	-3.0096866373	1.9866226741
C	3.119988719	-1.6225753479	-1.8615299983
C	3.4334645887	-0.5641050101	0.2953835864
H	3.6266869061	-2.9919351175	2.0840803802
H	2.0841389272	-2.1744121965	2.5256509372
H	2.158101951	-3.9475369711	2.4005699251
C	3.7731531138	-0.5572769782	-2.4792479293
H	2.7597068274	-2.458096592	-2.4563411152
C	4.1036043711	0.4895806265	-0.3331987973
H	3.2891070776	-0.5392084437	1.3698505426
C	4.2735425945	0.502267154	-1.7181806278
H	3.90394074	-0.5640730518	-3.5581793035
H	4.4884767238	1.3069613469	0.2711309809
H	4.791464638	1.326644216	-2.1997055087
C	-4.3595711759	-2.3539163619	-1.2069813829
C	-4.2623159773	-1.3286229311	-2.0629571684
C	-3.8853244992	-2.4977324193	0.21863013
H	-4.8677999803	-3.2452448648	-1.5781495306
C	-3.6231290576	0.0308618147	-1.8687710196
H	-4.6802779263	-1.4917131439	-3.0566979247
C	-2.8843620259	-1.4538824724	0.7574926172
H	-3.4374547733	-3.4968763692	0.3238782157
H	-4.7613124195	-2.5091622226	0.8860725215
C	-2.0939945935	0.0394896771	-2.0787356607
H	-3.8732393719	0.4619513521	-0.8961841634
H	-4.0485467847	0.7196514069	-2.6085263592
C	-1.5739847881	-1.4614293666	0.0024108769
H	-3.3403311548	-0.4622927968	0.7635972885
H	-2.6690357671	-1.6910606228	1.8048152025
C	-1.2493780503	-0.8104621764	-1.1542288727

H	-1.8846809525	-0.3233032805	-3.095186417
H	-1.7315101038	1.0747829063	-2.0540869302
H	-0.8503214803	-2.2020322793	0.3498829233
H	-0.2816007118	-1.0817079185	-1.5854468894
C	-0.3824513291	2.1442302489	0.2121226177
C	0.8049634068	2.8799472783	0.0329302927
C	-1.5908455168	2.8589613026	0.1162347924
C	0.7877064955	4.2489436383	-0.2549056309
H	1.7697489652	2.381631354	0.1163811956
C	-1.6210392079	4.2289140315	-0.1618721927
H	-2.5413217944	2.3462198802	0.2670954083
C	-0.4275020715	4.9286852947	-0.352730296
H	1.7237023693	4.7858852995	-0.3960338184
H	-2.5738962326	4.7504437795	-0.2272421835
H	-0.4450214056	5.9940340663	-0.5697049781

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9A^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.1975868877	-0.1757242916	0.3620185311
S	0.1722930029	-0.4823206634	2.5354352426
C	-0.481195355	0.9487052478	3.4809554687
H	-1.5608934662	0.8540899745	3.6332280499
H	0.0068957424	0.9621717488	4.4592714309
H	-0.2752184952	1.8880023904	2.9624768801
S	1.8386950087	-2.021454425	-0.4637071326
C	3.2702933035	-0.9385567042	-0.5842471481
C	2.2383239904	-2.9965836836	1.0383409558
C	4.1521258754	-1.1034649544	-1.6594320146
C	3.4915887543	0.0721495029	0.3612697163
H	3.2087335179	-3.481433635	0.911682168
H	2.2263155	-2.359441789	1.9247579125
H	1.4608829702	-3.7594982287	1.1338128767
C	5.2568786779	-0.2589636461	-1.7867766124
H	3.9725837174	-1.8897118315	-2.386549704
C	4.6064561883	0.9019873825	0.2327424528
H	2.7943663662	0.2070087615	1.1841658881
C	5.4873897502	0.7404642104	-0.8395432896
H	5.9389452739	-0.3875316047	-2.6228768064
H	4.7782888005	1.6836152738	0.967555209
H	6.3497393286	1.3942060506	-0.9380102701
C	-5.0393926576	-1.7842923538	-0.7232949319
C	-4.8033677834	-0.8880491646	-1.6901064153
C	-4.4094357539	-1.9574115513	0.6370519741
H	-5.8194419549	-2.5196737729	-0.9272925879
C	-3.8000846177	0.246330529	-1.7330622604
H	-5.3995861705	-0.9955302395	-2.5968094315
C	-3.1092494028	-1.183408774	0.9370582496
H	-4.2211174129	-3.0310988407	0.7869292361
H	-5.150835809	-1.6917841462	1.4071166973
C	-2.3739788757	-0.1955323755	-2.1207963743
H	-3.7729463661	0.8114640808	-0.7990145465
H	-4.1269164464	0.9642409809	-2.4947928307
C	-1.959149175	-1.5963763759	0.0467387149
H	-3.2890497657	-0.1089315081	0.8793894443
H	-2.8175944233	-1.3852165453	1.9731366811
C	-1.6548332608	-1.1610070109	-1.2070197453
H	-2.4188903458	-0.6896432856	-3.102379649
H	-1.7496511163	0.6954747534	-2.2647579761

H	-1.399917331	-2.4605392752	0.4094875246
H	-0.8464995686	-1.6972176692	-1.707389457
C	-0.3742905242	1.7010336649	-0.1236530102
C	0.5671861403	2.3043867293	-0.9819515993
C	-1.4214552802	2.5264427141	0.3291888491
C	0.4643818218	3.643599095	-1.3758620286
H	1.41399389	1.7297339434	-1.3576282628
C	-1.534911315	3.8672026938	-0.052775466
H	-2.1714301273	2.1253885444	1.0112199378
C	-0.590002017	4.4314276371	-0.9120666487
H	1.2117287648	4.0717698298	-2.0412756675
H	-2.3586947818	4.4717670763	0.3220091983
H	-0.6720258985	5.4734165305	-1.2121064227

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9B^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.3945672864	0.1551580964	0.049679952
S	-0.6071830878	-0.6485247554	2.1372689798
C	-1.1430532238	0.6313759318	3.3402052157
H	-2.2332631996	0.7224648338	3.367366348
H	-0.7991552315	0.3313427133	4.3340315158
H	-0.7067806989	1.6054870887	3.1003488114
S	1.0238404577	-1.9030738406	-0.8690498364
C	2.734317232	-1.5543256466	-0.4387470397
C	0.6660779161	-3.351092967	0.1989202407
C	3.7181919426	-1.7274595378	-1.4187181523
C	3.0790167582	-1.09842092	0.8395836872
H	1.3953439622	-4.1388266714	-0.001905963
H	0.6767270846	-3.0619271477	1.2515414953
H	-0.3341211569	-3.7026183029	-0.0668297438
C	5.0526114319	-1.4495791583	-1.1163475586
H	3.4384785226	-2.0785015164	-2.4074325566
C	4.4175223971	-0.8382398522	1.135724345
H	2.3058935219	-0.9447461396	1.5876458152
C	5.4036488681	-1.0100355757	0.1611777304
H	5.8158845568	-1.5818245971	-1.8783349974
H	4.6871593441	-0.4873614836	2.1280774419
H	6.443044733	-0.7974210936	0.3961369112
C	-5.2932278613	-0.9246691056	-1.0659913405
C	-5.3843259792	-0.1204250311	0.0007848134
C	-4.1382763618	-1.7302349224	-1.6055497554
H	-6.2015090955	-1.0420782545	-1.6594465567
C	-4.3263474345	0.2762921739	1.010426839
H	-6.3539631607	0.3530497981	0.1573729881
C	-2.7424213084	-1.5064325801	-0.9886929789
H	-4.0778667075	-1.5524667665	-2.6899162137
H	-4.385118902	-2.7993605487	-1.508127151
C	-3.3812679145	1.3819547117	0.5001110606
H	-3.7410958325	-0.5756014772	1.3648407168
H	-4.8355869941	0.6721609547	1.8973704394
C	-2.1768052827	-0.125667773	-1.2634106109
H	-2.7581693346	-1.7258176816	0.0797628197
H	-2.0656690934	-2.2428977663	-1.4398682052
C	-2.4538903737	1.0578492764	-0.6439843571
H	-3.9873633833	2.2361570516	0.1637509009
H	-2.7812859469	1.7697275916	1.3334139515
H	-1.6277872667	-0.044747729	-2.2054022939
H	-2.0350094758	1.9467601463	-1.1106179126

C	0.5997596825	1.8180428676	-0.1806002195
C	0.6113263577	2.5121592553	-1.4050414806
C	1.3813773104	2.363974959	0.8540155626
C	1.3560783209	3.6817526502	-1.5944094681
H	0.0318497012	2.1403718699	-2.2530858106
C	2.1223706431	3.5376037248	0.6840121739
H	1.4212834252	1.8611139498	1.8190521842
C	2.1127480731	4.2024277675	-0.5440564038
H	1.3424407835	4.1858901083	-2.5589863782
H	2.7111598922	3.9323269397	1.5100660878
H	2.6889456753	5.1145043815	-0.680815043

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$TS^{3}_{9B\text{-}9C}$ B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.362739716	0.110482935	0.0096820199
S	-0.530662994	-0.7387768429	2.0853782658
C	-1.1539602584	0.4817175178	3.3085840507
H	-2.2472543063	0.5244037014	3.3173082027
H	-0.8156045334	0.1700670851	4.3007545661
H	-0.7559329052	1.4808345423	3.1066419774
S	1.1216878738	-1.7961190732	-0.8853055437
C	2.8150664698	-1.4630248435	-0.38161666
C	0.755629804	-3.3328964665	0.0456648423
C	3.8205487502	-1.5200184936	-1.3527643762
C	3.1247201288	-1.1361793763	0.9440583696
H	1.503860253	-4.0905414921	-0.1967604529
H	0.7298148835	-3.1319098612	1.1183258861
H	-0.2301460102	-3.6746487494	-0.2801966979
C	5.1437875569	-1.2560709471	-0.9941057057
H	3.5666315856	-1.7702529617	-2.3783347221
C	4.4527546064	-0.8897134747	1.294378595
H	2.3331073416	-1.0682240074	1.6855998516
C	5.4613794107	-0.9463616745	0.3293409013
H	5.9243620527	-1.2976066093	-1.7488283998
H	4.6964745211	-0.6394562988	2.3233075884
H	6.4922405589	-0.7450197944	0.6078682261
C	-5.350346868	-0.8485185175	-1.039938289
C	-5.420304955	-0.0629988117	0.0422307702
C	-4.2109926956	-1.6587196278	-1.6053614699
H	-6.2655244704	-0.9422385908	-1.6269307512
C	-4.3468070276	0.2981944274	1.0487519633
H	-6.3811954319	0.4216170463	0.2173171486
C	-2.8054882986	-1.4582735878	-1.0023808404
H	-4.1619968943	-1.4646627479	-2.6874706942
H	-4.4680938112	-2.7265319887	-1.5211574309
C	-3.3940457236	1.4043034782	0.5533064302
H	-3.7687312683	-0.5698887283	1.3744061848
H	-4.8410922311	0.6779563824	1.9510768019
C	-2.2321646326	-0.0765088915	-1.2550007529
H	-2.8075463135	-1.7004086711	0.0611698847
H	-2.1405937349	-2.1912269883	-1.4768646682
C	-2.489416589	1.0956005823	-0.6119989658
H	-3.9925187512	2.2763627973	0.2508741946
H	-2.7764147255	1.7606411725	1.388218084
H	-1.6808412958	0.0170251787	-2.1949896589
H	-2.048943562	1.9864458423	-1.0553867354
C	0.6646004021	1.7387968028	-0.3011568389
C	0.640926525	2.415794437	-1.5350245057

C	1.477899042	2.2970052747	0.7020624094
C	1.3836694732	3.579786394	-1.7635761475
H	0.0351857568	2.0333930683	-2.3597755333
C	2.2178434963	3.4648264205	0.49270996
H	1.5435934795	1.8079575037	1.6728271274
C	2.1738828911	4.1119881052	-0.7441428725
H	1.3424948997	4.0704904627	-2.734337609
H	2.8325388978	3.8692628318	1.294865118
H	2.7496123429	5.0192941286	-0.9114860978

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9C^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.3299859426	0.1628620252	0.3641303547
S	-0.5355119773	-0.8826978771	2.3312965193
C	-1.1881694654	0.3508520351	3.5338173137
H	-2.236832609	0.593172086	3.335576487
H	-1.1188957226	-0.0803821512	4.5359821914
H	-0.6018543429	1.2746413197	3.5148296489
S	0.9005860781	-1.5846502055	-0.8090135129
C	2.6367509487	-1.3332192418	-0.4124848912
C	0.5962189742	-3.2100014942	-0.0162390712
C	3.5667951987	-1.3755342594	-1.4559805306
C	3.0507031331	-1.0926142105	0.9027296151
H	1.2894426792	-3.9440059401	-0.4325640916
H	0.707596819	-3.1338797495	1.0666993384
H	-0.4309434096	-3.4968886635	-0.2528178091
C	4.9222340424	-1.1857729045	-1.1800839104
H	3.2308751012	-1.5546086489	-2.4727966667
C	4.4089544291	-0.916244244	1.1683994598
H	2.317495224	-1.0399524342	1.7030718175
C	5.3439611394	-0.960432048	0.1311663675
H	5.6456624041	-1.2158303876	-1.9901453853
H	4.7345870568	-0.7323040465	2.1885059479
H	6.3993614016	-0.8145759041	0.3446199968
C	-5.3934168052	-0.9085331137	-1.1388627764
C	-5.4608680582	-0.0659337771	-0.1005998348
C	-4.2577683036	-1.7580035704	-1.6521469436
H	-6.3055349639	-1.0228752697	-1.7269374696
C	-4.3880016153	0.3272755469	0.893650363
H	-6.4158851071	0.4399847777	0.0434903862
C	-2.8463643427	-1.5149161334	-1.0771637652
H	-4.2158492965	-1.6378192554	-2.7450124338
H	-4.5147348292	-2.8174106405	-1.4932541665
C	-3.4189317453	1.4003904252	0.3577242511
H	-3.8232776101	-0.5346172494	1.2576830089
H	-4.8806560583	0.7494537912	1.7779315031
C	-2.2831912887	-0.1464014031	-1.4000665121
H	-2.834886685	-1.7078618068	-0.0023242218
H	-2.1827584723	-2.2658940997	-1.5242269435
C	-2.5279880543	1.0416986753	-0.8070180398
H	-4.000791632	2.2803403697	0.0468831545
H	-2.7873009514	1.7628066065	1.1836982034
H	-1.6558306307	-0.1105442558	-2.291506069
H	-2.0404429265	1.9068860327	-1.2538883156
C	0.7105346897	1.7160885821	-0.1713771587
C	0.7763611311	2.2034160784	-1.4907087198
C	1.4356798356	2.4398802423	0.7939451419
C	1.509010249	3.3450554682	-1.8318246297

H	0.2474773662	1.681424346	-2.2902635022
C	2.1666887701	3.587959445	0.4726798511
H	1.4427756101	2.0994917271	1.8295740882
C	2.2058488507	4.0456234635	-0.8457409573
H	1.5363414295	3.6872079116	-2.8647893056
H	2.7099990719	4.1228695818	1.2494378505
H	2.7756702122	4.9356104486	-1.1025332259

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$TS^{3}_{9C\text{-}10}$ B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.083750551	0.0206063149	0.5021532926
S	-0.3160478218	-1.355711688	2.2079707885
C	-1.2131026424	-0.4305340485	3.5238872401
H	-2.2000812651	-0.1010993414	3.1881650326
H	-1.3412583072	-1.101517104	4.3770247333
H	-0.63699331	0.4400609842	3.850678536
S	1.0907498023	-1.3738334523	-1.0610880819
C	2.8302603756	-1.2334497666	-0.626506972
C	0.757562454	-3.1347940915	-0.6775376683
C	3.7537166482	-1.0322045152	-1.6576007075
C	3.2539467842	-1.3066014927	0.7058447307
H	1.4142945069	-3.7617303289	-1.2843396292
H	0.8995220449	-3.3321743021	0.3863171048
H	-0.2850066212	-3.324555571	-0.9428478098
C	5.1112306229	-0.9134088998	-1.3542476611
H	3.4106664856	-0.9682906459	-2.6856610703
C	4.6142339205	-1.1969418166	0.9962536582
H	2.5297239998	-1.4415122234	1.5047315556
C	5.5420661669	-0.9993413803	-0.0293994792
H	5.8292638345	-0.7549383075	-2.1539861884
H	4.9465280566	-1.2555183443	2.0289337382
H	6.5990632128	-0.907663464	0.2048505963
C	-5.4082549718	-0.7959070449	-0.175981913
C	-5.0572925904	0.3679665919	0.3844975802
C	-4.5776352679	-1.884474927	-0.8069674121
H	-6.4760525249	-1.0222270351	-0.1848938731
C	-3.6866050537	0.9917240547	0.5385606221
H	-5.8748440815	0.9843493491	0.7597636805
C	-3.0768980653	-1.62032792	-1.0467641316
H	-5.0441778718	-2.1450292309	-1.7691636914
H	-4.6731603367	-2.7920019511	-0.1896018009
C	-3.1688186628	1.681594684	-0.7395140028
H	-2.9436579809	0.2676449199	0.8885147584
H	-3.7440352375	1.7558242922	1.3234279516
C	-2.7785418821	-0.526560944	-2.0546800505
H	-2.5721436588	-1.4458517161	-0.0921637439
H	-2.6489746963	-2.5553769308	-1.4318529622
C	-2.8268918849	0.8076669212	-1.9197987648
H	-3.9170128568	2.4163885411	-1.0727431911
H	-2.2769353555	2.2754700763	-0.4876573631
H	-2.5137627714	-0.8914755764	-3.0476707166
H	-2.5762715663	1.3850913391	-2.8115080897
C	0.6677262892	1.7672035325	0.1618769993
C	0.6947536868	2.3397848539	-1.1252304645
C	1.1827913971	2.5508049835	1.2110844138
C	1.1958758839	3.6257915826	-1.3535652973
H	0.3139048503	1.7778439633	-1.9783194583
C	1.6877184279	3.8365631419	0.9970157988

H	1.2027803411	2.1518260929	2.2251108533
C	1.695365088	4.3789249437	-0.2897984943
H	1.1994315453	4.0375120575	-2.3609695435
H	2.0784755675	4.4142093007	1.8323606172
H	2.0894408432	5.3777435393	-0.4619770497

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10^3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-0.083750551	0.0206063149	0.5021532926
S	-0.3160478218	-1.355711688	2.2079707885
C	-1.2131026424	-0.4305340485	3.5238872401
H	-2.2000812651	-0.1010993414	3.1881650326
H	-1.3412583072	-1.101517104	4.3770247333
H	-0.63699331	0.4400609842	3.850678536
S	1.0907498023	-1.3738334523	-1.0610880819
C	2.8302603756	-1.2334497666	-0.626506972
C	0.757562454	-3.1347940915	-0.6775376683
C	3.7537166482	-1.0322045152	-1.6576007075
C	3.2539467842	-1.3066014927	0.7058447307
H	1.4142945069	-3.7617303289	-1.2843396292
H	0.8995220449	-3.3321743021	0.3863171048
H	-0.2850066212	-3.324555571	-0.9428478098
C	5.1112306229	-0.9134088998	-1.3542476611
H	3.4106664856	-0.9682906459	-2.6856610703
C	4.6142339205	-1.1969418166	0.9962536582
H	2.5297239998	-1.4415122234	1.5047315556
C	5.5420661669	-0.9993413803	-0.0293994792
H	5.8292638345	-0.7549383075	-2.1539861884
H	4.9465280566	-1.2555183443	2.0289337382
H	6.5990632128	-0.907663464	0.2048505963
C	-5.4082549718	-0.7959070449	-0.175981913
C	-5.0572925904	0.3679665919	0.3844975802
C	-4.5776352679	-1.884474927	-0.8069674121
H	-6.4760525249	-1.0222270351	-0.1848938731
C	-3.6866050537	0.9917240547	0.5385606221
H	-5.8748440815	0.9843493491	0.7597636805
C	-3.0768980653	-1.62032792	-1.0467641316
H	-5.0441778718	-2.1450292309	-1.7691636914
H	-4.6731603367	-2.7920019511	-0.1896018009
C	-3.1688186628	1.681594684	-0.7395140028
H	-2.9436579809	0.2676449199	0.8885147584
H	-3.7440352375	1.7558242922	1.3234279516
C	-2.7785418821	-0.526560944	-2.0546800505
H	-2.5721436588	-1.4458517161	-0.0921637439
H	-2.6489746963	-2.5553769308	-1.4318529622
C	-2.8268918849	0.8076669212	-1.9197987648
H	-3.9170128568	2.4163885411	-1.0727431911
H	-2.2769353555	2.2754700763	-0.4876573631
H	-2.5137627714	-0.8914755764	-3.0476707166
H	-2.5762715663	1.3850913391	-2.8115080897
C	0.6677262892	1.7672035325	0.1618769993
C	0.6947536868	2.3397848539	-1.1252304645
C	1.1827913971	2.5508049835	1.2110844138
C	1.1958758839	3.6257915826	-1.3535652973
H	0.3139048503	1.7778439633	-1.9783194583
C	1.6877184279	3.8365631419	0.9970157988
H	1.2027803411	2.1518260929	2.2251108533
C	1.695365088	4.3789249437	-0.2897984943

H	1.1994315453	4.0375120575	-2.3609695435
H	2.0784755675	4.4142093007	1.8323606172
H	2.0894408432	5.3777435393	-0.4619770497

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CP3 B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	-1.01274	-0.74738	-0.21003
S	-1.68751	-2.38822	1.0157
C	-3.34777	-2.90557	0.40502
H	-3.31272	-3.24929	-0.63249
H	-3.70051	-3.72712	1.03345
H	-4.05867	-2.07894	0.48313
S	0.98497	-0.6578	-1.40494
C	2.25921	-0.08724	-0.27267
C	1.48175	-2.40473	-1.66113
C	3.25514	0.76195	-0.76567
C	2.2573	-0.473	1.07315
H	2.47235	-2.4341	-2.12042
H	1.47394	-2.95063	-0.71602
H	0.74867	-2.84628	-2.34066
C	4.261	1.21541	0.08974
H	3.23969	1.06335	-1.80839
C	3.27049	-0.02116	1.91857
H	1.47122	-1.11685	1.4567
C	4.2721	0.82075	1.42855
H	5.03493	1.87506	-0.29239
H	3.27177	-0.3228	2.96203
H	5.05711	1.17286	2.092
C	-1.49701	1.08295	-0.11162
C	-1.44641	1.92297	-1.23795
C	-1.95959	1.64075	1.09269
C	-1.83287	3.26534	-1.16727
H	-1.09719	1.53736	-2.19519
C	-2.34622	2.98165	1.17273
H	-2.02449	1.021	1.98434
C	-2.28077	3.79919	0.04198
H	-1.78177	3.89168	-2.05544
H	-2.6971	3.3888	2.11891
H	-2.57825	4.84314	0.10261

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$TS_{2\text{-}25}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.6799719788	-0.3427052833	-0.4707581408
C	2.1953201098	0.8954342817	-1.0195059812
C	1.618399831	1.3346185549	0.1793886622
C	2.1871667066	1.1276010879	1.5715354681
C	2.7107439273	-0.3089991548	1.8123117002
C	1.8840515595	-1.3582923384	1.0893692941
C	2.1479046444	-1.8672351786	-0.1615228928
C	3.2682141533	-1.4318780743	-1.0858309149
C	3.4944200073	0.1011551524	-1.131989784
H	1.9296514062	1.4471118272	-1.917509791
H	0.9437768061	2.1882789077	0.094636465
H	1.3903981701	1.3355539978	2.2972298382
H	2.98217397	1.8606488302	1.7861104637
H	3.760462233	-0.3871831036	1.512330958
H	2.694821085	-0.5217463021	2.8882430147

H	1.1896383674	-1.9202433925	1.7072657843
H	1.6803301384	-2.8130221065	-0.4275862739
H	3.0203877013	-1.7810195323	-2.0948108504
H	4.205790137	-1.9408334939	-0.8107220221
H	4.1908692614	0.4086922368	-0.3447236596
H	3.9860395504	0.3524351484	-2.0789933853
C	-1.6451429161	0.4236158573	0.8167810397
C	-1.5375895279	-0.9077161028	1.0241574198
C	-1.5948598769	1.5786250495	1.7910849299
H	-1.9515995135	0.7229082781	-0.1826805009
C	-1.3449262622	-1.6514805281	2.3269837516
H	-1.7827680324	-1.5462837536	0.1785468979
C	-1.7140639904	1.2669098681	3.299287863
H	-2.4180656965	2.2546293284	1.5181176001
H	-0.6810816617	2.1650508854	1.6227009601
C	-2.6681474032	-1.8728552205	3.0918122552
H	-0.6174095481	-1.1618991416	2.9764178573
H	-0.9291490932	-2.6418059231	2.1033961013
C	-3.0286912956	0.6228908143	3.688107601
H	-0.8589686024	0.6717284786	3.6300062065
H	-1.6287179421	2.2213274913	3.8335255296
C	-3.4093701996	-0.6572470784	3.5917275762
H	-3.353804397	-2.4409143064	2.4455024915
H	-2.4686273004	-2.5388924378	3.9467419846
H	-3.7740014053	1.3176285061	4.0764523899
H	-4.4208745487	-0.8861635106	3.9314600343
Si	-0.4378583817	-0.0321293651	-2.4739374675
H	-0.0561560431	-1.3261326191	-1.3684706504
C	-2.1854937268	-0.7579609449	-2.7394056355
H	-2.1606840344	-1.8478312511	-2.8624091733
H	-2.8553883439	-0.5410801416	-1.8973109004
H	-2.6524135893	-0.3327274244	-3.6374020393
C	0.6122539164	-0.517874188	-3.9853153618
H	0.1297387475	-0.1895626433	-4.9150407797
H	1.6117811938	-0.0683520246	-3.9568121586
H	0.7387737965	-1.6057675485	-4.0424728876
C	-0.765581385	1.8571162487	-2.6228769372
H	-1.469643743	2.2158280968	-1.8626738733
H	0.1379531629	2.4724259139	-2.5505097616
H	-1.2211707206	2.0558404424	-3.6032289047

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25 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.027307	0.131555	-0.362761
C	0.960621	0.187023	1.473937
C	0.787949	-1.123921	1.055899
C	1.813547	-1.994413	0.357123
C	2.697336	-1.238871	-0.672098
C	1.915684	-0.201381	-1.451833
C	1.793816	1.124856	-1.13888
C	2.353407	1.823643	0.081537
C	2.250375	0.991212	1.388041
H	0.219926	0.574599	2.17157
H	-0.046278	-1.67698	1.48517
H	1.272101	-2.79528	-0.162192
H	2.45645	-2.497875	1.095889
H	3.551681	-0.774089	-0.172355
H	3.117974	-1.968307	-1.373851

H	1.550334	-0.515914	-2.428331
H	1.378601	1.781986	-1.901128
H	1.793978	2.75771	0.21345
H	3.399122	2.122401	-0.088703
H	3.117259	0.331237	1.488303
H	2.297329	1.677762	2.241029
Si	-2.210062	0.034468	-0.057813
H	-0.893816	0.475425	-1.4908
C	-2.938779	-1.538653	-0.855506
H	-2.871353	-1.497363	-1.948763
H	-2.414015	-2.443933	-0.525305
H	-3.996921	-1.656213	-0.586522
C	-3.249313	1.527163	-0.631714
H	-4.288949	1.445031	-0.287987
H	-2.847185	2.468568	-0.23545
H	-3.256441	1.6095	-1.724813
C	-2.59763	-0.095479	1.820947
H	-2.10874	-0.949366	2.305619
H	-2.296366	0.811129	2.360843
H	-3.680501	-0.213193	1.96629

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$TS_{25\text{-}26}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.4003949692	-0.3647762965	-0.2929701579
Si	-1.336925225	-2.4917425924	0.6743614678
H	-1.9279653343	-1.7097546762	-0.6998258057
C	0.4914591893	-3.0125727217	0.6016402247
C	-2.3469618931	-4.0280760741	0.182343468
C	-1.9002402173	-2.0628584441	2.4416153378
H	1.173113724	-2.2463602216	0.9825163331
H	0.6382887196	-3.9224904711	1.198868099
H	0.7874121872	-3.2458901592	-0.4281053443
H	-2.1763744318	-4.8572312625	0.881105102
H	-3.4220009704	-3.8096377408	0.1835117837
H	-2.0844026782	-4.3792640848	-0.822888157
H	-1.3119853888	-1.2575100651	2.8882022504
H	-2.9526926734	-1.7554036601	2.4480639162
H	-1.8145669273	-2.9526129722	3.0805734193
C	-0.8377823512	1.3967039715	-1.0070043575
C	-1.9876971542	1.4993803869	-0.2021694752
C	0.574222615	1.8999380384	-0.7175687538
H	-1.039984485	1.3009009058	-2.0770248421
C	-2.1648398774	2.1584264276	1.1547684857
H	-2.9383554601	1.4662955407	-0.7457030969
C	1.421686864	1.0093562832	0.212290005
H	0.5521386722	2.9280872898	-0.3401944297
H	1.110892358	1.955613578	-1.6726939196
C	-0.8952583801	2.490133503	1.9695905721
H	-2.8280411959	1.5291035175	1.7666361928
H	-2.7175054092	3.0989264853	1.0003158163
C	0.8792659341	0.6752127039	1.5808124829
H	1.6079700208	0.0581900073	-0.3064958404
H	2.416647011	1.4679283926	0.3329215405
C	-0.0571796967	1.2862764789	2.3210075769
H	-0.305378286	3.2398831753	1.4369778611
H	-1.2191264928	2.9717556083	2.9007406293
H	1.3652149006	-0.1868914522	2.0395226996
H	-0.2691825083	0.8472544405	3.2962371458

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26 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.5820081735	-0.1823135157	-0.9846536194
Si	-0.4358241184	-2.1879872423	0.1429304159
H	-1.0474385169	-1.5852502654	-1.3074066748
C	1.4126292115	-2.6321508463	0.134712753
C	-1.3744114	-3.8069768356	-0.2034005503
C	-1.0352160589	-1.6101159069	1.8532739069
H	2.0451230917	-1.8205672416	0.5055980256
H	1.5779014208	-3.5094627191	0.7744311124
H	1.7512195207	-2.8940895418	-0.874642365
H	-1.1804144794	-4.5564696946	0.5748551547
H	-2.4573943968	-3.6342278385	-0.2338738412
H	-1.0843331653	-4.2435718541	-1.1668467532
H	-0.4627653839	-0.7567649326	2.2255766249
H	-2.0929694934	-1.3238862386	1.8195328872
H	-0.9408042256	-2.4352184359	2.5729457525
C	0.0593775408	1.6176858243	-1.4480764996
C	-1.0767674265	1.6706605788	-0.6173717393
C	1.4861529786	2.0936488386	-1.1842982567
H	-0.1768206117	1.6217026454	-2.5184699294
C	-1.2332178597	2.2296419717	0.7881542092
H	-2.0325689756	1.7043127988	-1.1550204666
C	2.35838675	1.2362440158	-0.2505387744
H	1.4853855965	3.1359539032	-0.8437279757
H	2.0031447981	2.1104479862	-2.1518668553
C	0.032138764	2.7324772853	1.5156026312
H	-1.7489294755	1.4941534721	1.4219869967
H	-1.9252701642	3.082941954	0.7143915409
C	1.9529437314	1.0501538065	1.1891984583
H	2.4493681665	0.2359229781	-0.6985347286
H	3.3814145216	1.6462813438	-0.2640767249
C	1.0098335269	1.6551002194	1.9229700446
H	0.5165305155	3.4982359659	0.9040126116
H	-0.3017656079	3.2475593516	2.4250330918
H	2.5493307641	0.2936634161	1.70283332
H	0.9147546342	1.3208037532	2.9567192172

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PhSMe B3LYP/BSI Optimized geometry (charge = 0 , singlet)

S	-1.8952066516	0.0546722721	-0.6555759467
C	-0.1479673324	-0.0466006862	-0.3075001476
C	0.5645090809	-1.2445552706	-0.1678849623
C	0.5335433151	1.1746522155	-0.1691722104
C	1.935063528	-1.2161732446	0.1053961477
H	0.0659936701	-2.202298325	-0.2691904778
C	1.8987193422	1.1919999438	0.103030703
H	-0.0102101436	2.1099421233	-0.2756965608
C	2.6093572866	-0.0039448271	0.2422783294
H	2.4735347009	-2.1546241215	0.2108456326
H	2.4096743504	2.1456907998	0.2068209117
H	3.6745004773	0.0116347078	0.4546535673
C	-2.4136878324	-1.688542159	-0.7628983415
H	-2.2542167093	-2.2160696931	0.1817086365
H	-3.4853357935	-1.6645649895	-0.9766303458
H	-1.9035137188	-2.2121366056	-1.5762690253

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HSiMe$_3$ B3LYP/BSI Optimized geometry (charge = 0 , singlet)

Si	-0.0001645875	0.0000368265	0.3770141641
H	-0.0002119143	-0.0000998472	1.8726495605
C	-1.1795880785	-1.3550192211	-0.2206745137
H	-1.2164815949	-1.3966905032	-1.3162958959
H	-0.8658296858	-2.3424677871	0.1382734213
H	-2.2006944073	-1.1809857527	0.139037732
C	-0.5838892286	1.6990621808	-0.2204542399
H	0.0770777574	2.4963330881	0.1398511898
H	-0.6008929186	1.7521061786	-1.3160719281
H	-1.5961600458	1.9208301089	0.1379718088
C	1.7631632761	-0.3438592359	-0.2204353126
H	2.4613620747	0.421660978	0.1385115157
H	2.1229865879	-1.3151203803	0.1394520656
H	1.8178927653	-0.3551266334	-1.3160495674

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COD B3LYP/BSI Optimized geometry (charge = 0 , singlet)

C	1.2139093548	-1.2394618961	-0.4926256836
C	-0.0093989302	-1.7067210764	-0.2133452986
C	1.9231777645	0.0099144254	-0.0299485567
H	1.8206555446	-1.8492476591	-1.1644823667
C	-1.0868165406	-1.1063144403	0.6650712415
H	-0.2912064089	-2.6402381179	-0.7016721466
C	1.0868288039	1.1063398051	0.6650217316
H	2.4168531446	0.4542683443	-0.9071678745
H	2.7472314223	-0.281719901	0.6414268072
C	-1.9231682712	-0.0099173292	-0.0299403324
H	-0.6735397959	-0.7217723671	1.6008437642
H	-1.777470002	-1.9072375128	0.9575832629
C	0.0094075962	1.7067107426	-0.2134147624
H	0.6735558937	0.7218358032	1.6008115714
H	1.7774834461	1.9072747711	0.957498416
C	-1.2139018648	1.2394402506	-0.4926711025
H	-2.4168471049	-0.4543069564	-0.9071396041
H	-2.7472192858	0.2817442733	0.6414264204
H	0.2912130737	2.6402080291	-0.7017805473
H	-1.8206508399	1.8491988118	-1.1645499396

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Me$_3$SiSMe B3LYP/BSI Optimized geometry (charge = 0 , singlet)

Si	-0.6599409939	-0.0544346373	-0.0000706236
S	1.2843836941	0.917521956	-0.0003800299
C	2.4447882141	-0.5158025943	0.000067518
H	2.320312102	-1.1325834082	-0.8936981342
H	3.4554221227	-0.1011195986	-0.0000555371
H	2.3203035504	-1.132031874	0.894212323
C	-0.8747315704	-1.1258396872	-1.5456325546
H	-0.1316817878	-1.9305201485	-1.5936706535
H	-1.8668211233	-1.5958305499	-1.5523467868
H	-0.7786333906	-0.5258330461	-2.4572607587
C	-0.8747067313	-1.1249068978	1.5461414094
H	-0.7785671034	-0.5243557203	2.4574065931
H	-1.8668071751	-1.5948701438	1.5531684779

H	-0.1316745906	-1.9295760153	1.5946391703
C	-1.9014386979	1.3689194933	-0.0004902581
H	-1.7841195932	2.0023977914	-0.8867568541
H	-2.9275987271	0.9803526729	-0.000382722
H	-1.7841281987	2.0029124077	0.8854094209

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benzene B3LYP/BSI Optimized geometry (charge = 0 , singlet)

C	0.9087126268	-1.0617187076	0.0000082143
C	-0.4645431881	-1.31774513	0.0000102971
C	-1.3729127377	-0.2564544809	0.0000128914
C	-0.9079693124	1.0608515897	0.00001167
C	0.4653242037	1.3168640698	0.0000086627
C	1.3736598495	0.2555417626	0.0000077797
H	1.6155006082	-1.8875209327	0.0000074232
H	-0.8263005445	-2.3427774613	0.0000106718
H	-2.4414987847	-0.4556525806	0.0000152522
H	-1.6147767767	1.8866743528	0.0000130631
H	0.8271118805	2.3418844309	0.0000083864
H	2.4422521755	0.4547130873	0.000005688

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1T B3LYP/BSI Optimized geometry (charge = 0 singlet)

Ni	0.1054867446	-0.6379167561	0.6591137553
S	-2.5986880763	-0.1123321978	-0.6251018901
C	-1.7981097478	-0.5646672562	0.9297923408
C	-4.3775361774	-0.3175885066	-0.2088552896
C	-2.0062753915	0.2624409425	2.0889284666
C	-1.2842685305	-1.9052025032	1.1329500387
H	-4.9454425263	-0.045024858	-1.1033452699
H	-4.5961090611	-1.3561959995	0.0538780828
H	-4.6684087983	0.3398573778	0.6147078306
C	-1.7584675694	-0.2110458239	3.3604562652
H	-2.3929094299	1.2684670321	1.9438930341
C	-1.0531569419	-2.3558819445	2.4732119536
H	-1.4049938191	-2.6547796709	0.3518371422
C	-1.2799398581	-1.5330488969	3.5566550741
H	-1.928126306	0.4340864372	4.2189778403
H	-0.7241453003	-3.3811915124	2.6293716749
H	-1.1013418422	-1.8967549003	4.5652061017
S	2.1202982355	-0.2360432203	0.0916045667
C	2.1045360504	0.6515309704	-1.4771754166
C	3.0100991103	0.9798646865	1.1530583712
C	0.93686926	1.2948117482	-1.9013923992
C	3.250428275	0.665513943	-2.279901122
H	4.0105872387	1.1486410945	0.7473500265
H	2.4638463738	1.923210897	1.214343886
H	3.0883183473	0.5322261489	2.146816922
C	0.9214939956	1.9628427438	-3.1262045012
H	0.0554573696	1.2578021241	-1.2688912646
C	3.2299616955	1.3417065166	-3.5006606646
H	4.1472512556	0.1450659365	-1.955511658
C	2.0668835602	1.989731236	-3.9246254968
H	0.0124043054	2.4586771787	-3.4545469179
H	4.119509807	1.3538166188	-4.1246549971
H	2.052794752	2.509526414	-4.878705486

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$TS_{1T\text{-}10B}$ B3LYP/BSI Optimized geometry (charge = 0 singlet)

Ni	-0.596042043	-0.4505087159	-0.7371890056
S	-2.7213369176	-0.0412239114	-0.9308454365
C	-1.8097165473	-0.4865119974	0.6902294444
C	-3.6131722081	-1.5861508275	-1.3793615996
C	-1.858751559	0.4751763579	1.7350393534
C	-1.3830218612	-1.8110484642	0.9995406702
H	-4.6526100019	-1.3182453737	-1.5853799264
H	-3.1721052011	-2.0576340094	-2.2601256007
H	-3.5825713842	-2.2813482445	-0.5363489118
C	-1.4336997703	0.143739489	3.0123854394
H	-2.2175841161	1.4781132071	1.5207954416
C	-0.9691546654	-2.1203745093	2.3063859593
H	-1.4632688795	-2.6157752508	0.274848239
C	-0.9811769605	-1.1551920581	3.3082065403
H	-1.4663006005	0.8965330312	3.7965883623
H	-0.6401144875	-3.1328956747	2.5305819555
H	-0.6657124478	-1.4067927077	4.3168799724
S	1.4680244604	-0.6478775081	-1.2494432984
C	1.999935386	0.5541723321	-2.4877523439
C	2.4527871458	-0.1029942169	0.2075524099
C	1.026942044	1.3634421671	-3.0783220611
C	3.3309407009	0.6255080305	-2.9125642043
H	3.5173139952	-0.2598607586	0.0186118749
H	2.2594104125	0.946371666	0.4383553226
H	2.1313727202	-0.7261272396	1.0452557318
C	1.3844475229	2.2575467822	-4.0878775491
H	0.0032332844	1.2596755939	-2.7256365207
C	3.6858610841	1.5327728774	-3.9119767545
H	4.0831520055	-0.0234516056	-2.4725007701
C	2.715088425	2.3479151395	-4.5015276699
H	0.6250726734	2.8864287942	-4.5448527049
H	4.7204445813	1.5949511867	-4.2390866855
H	2.9965606396	3.0472284585	-5.2841136239

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10B B3LYP/BSI Optimized geometry (charge = 0 singlet)

Ni	-0.7849202405	-0.061939917	-0.0216758038
S	-2.7492782976	0.3683387237	-0.6031507119
C	-0.9004212773	-0.6834077195	1.7163332776
C	-3.5638082233	-1.2236909479	-1.0464657776
C	-1.3412164751	0.1410156365	2.7639159882
C	-0.5351736856	-2.0057618234	2.0173235512
H	-4.5818048503	-1.0010945137	-1.377077216
H	-3.0379451604	-1.7470776559	-1.849322138
H	-3.6143940675	-1.8715289003	-0.1673421641
C	-1.3911001873	-0.3373821307	4.0772422361
H	-1.6636608252	1.1582188301	2.5592218999
C	-0.5943935497	-2.4860524563	3.3301438751
H	-0.1973242279	-2.6756744072	1.2291913126
C	-1.0188969736	-1.6522106746	4.3657783283
H	-1.7359322468	0.3180536915	4.8741422594
H	-0.3050650976	-3.5135496758	3.5401567704
H	-1.0646593867	-2.0241890685	5.3861322427
S	1.4403109627	-0.2105215654	-0.0822664515
C	1.9618515814	0.6134031445	-1.5993848395

C	2.1064374618	0.9275575825	1.1926361224
C	1.0137619849	1.2282865716	-2.4229616676
C	3.3111751479	0.5866167498	-1.9712592856
H	3.1971438166	0.8801200266	1.1871579454
H	1.7673130707	1.9493385705	1.0117819297
H	1.7180530914	0.5721561832	2.1491995337
C	1.4208918728	1.8294832116	-3.6152134911
H	-0.0365152613	1.2308435893	-2.1390913551
C	3.7117051561	1.2016541308	-3.1574223525
H	4.0401073888	0.0848948154	-1.3410384228
C	2.7679395769	1.8223533604	-3.9804089703
H	0.6821879479	2.3052264522	-4.253862825
H	4.7595306569	1.1859841359	-3.4440985521
H	3.0826733168	2.29377705	-4.9071712479

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C1$_1$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.4060319161	0.2659390862	0.6203564574
S	-2.5603663458	1.6645355855	-2.2161334364
C	-1.757087707	1.7493339997	-0.6332134413
C	-3.8272108179	0.3737325072	-1.9724440723
C	-2.3244227776	1.2930350004	0.5824066985
C	-0.4805617904	2.3370951511	-0.5828799813
H	-3.3766660822	-0.551534747	-1.6035115501
H	-4.6251789294	0.7033546312	-1.3020447749
H	-4.2550360613	0.1928735025	-2.9618515
C	-1.6750980118	1.5173383389	1.8183835544
H	-3.2862934961	0.7977149351	0.5865877056
C	0.1707761092	2.5432290907	0.6507698511
H	0.0125129475	2.6330664697	-1.5027358203
C	-0.4312754672	2.175537346	1.8623870138
H	-2.1551054668	1.1871722102	2.7329129404
H	1.1604691958	2.98751928	0.6504928057
H	0.0697423643	2.3532844908	2.8071128915
Si	-1.0639217799	-1.8188281398	1.0371737828
C	-2.8708598892	-1.8603250386	1.6987668315
C	-1.1283410325	-2.9531814006	-0.5007887517
C	-0.0880858532	-2.7133536439	2.4143414002
H	-3.004612393	-1.2555689357	2.6046235073
H	-3.6058075827	-1.5218104744	0.9578544684
H	-3.1353684178	-2.8938644408	1.961655003
H	-1.8189075947	-2.5528745275	-1.2545159374
H	-1.4909181194	-3.9530014632	-0.2256362432
H	-0.1535483588	-3.0752287412	-0.9851915083
H	-0.4994327102	-3.7186618725	2.5782163956
H	0.978241913	-2.824033044	2.1911810173
H	-0.1731700368	-2.1674986682	3.3626074272
C	1.2946278696	-0.5947001511	0.149707905
H	1.9978753687	-0.51869348	2.1762921014
C	2.3331540148	-0.152401277	1.1975420247
C	1.6113176626	-0.2338695271	-1.3204092266
H	1.279991641	-1.6909177401	0.1869176567
H	2.3659319539	0.9418266366	1.2797031718
C	3.7949936589	-0.6514761201	0.9757362071
C	2.7512216387	-1.0580336876	-1.9907475937
H	1.8477393166	0.835866172	-1.4017321324
H	0.7009308278	-0.3836797467	-1.9130785521
C	4.6538938941	0.2861086694	0.1565019411

H	3.7754269436	-1.6597978525	0.5490553247
H	4.2710877291	-0.7550364533	1.9592878721
C	4.0340170773	-0.26894209	-2.2984352594
H	2.9831105032	-1.9392713287	-1.3829583961
H	2.3888285818	-1.4553671354	-2.9482907499
C	4.743077811	0.4410191172	-1.1707569856
H	3.7927818718	0.4916753	-3.0576764061
H	5.4428382415	1.2036929239	-1.5185914747
H	5.2733296652	0.9571973725	0.754201694
H	4.7532888368	-0.9390780903	-2.7974078562

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TS_{C1a} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-3.870821223979	1.999538834628	-7.056834708374
S	-6.755717763405	1.768218923450	-7.701786421878
C	-5.511365504397	2.999697420383	-7.297320298243
C	-8.276754462434	2.155994784965	-6.730349192461
C	-4.953507155742	3.080161025217	-5.938796198810
C	-5.498862485317	4.163488388470	-8.150361566883
H	-8.062678599911	2.147248325556	-5.659756210665
H	-8.599466063287	3.153210903856	-7.037020562244
H	-9.045857489270	1.421062383836	-6.976484191902
C	-4.450424438901	4.375838561144	-5.532765529026
H	-5.382750902654	2.480387381707	-5.133214918377
C	-4.902824568724	5.322783565070	-7.731589974338
H	-5.939731954302	4.097217376020	-9.142861927884
C	-4.382440882930	5.430797023730	-6.400930316045
H	-4.119358534303	4.497606100160	-4.503699019134
H	-4.848564239731	6.176717917426	-8.401023336944
H	-3.970592416782	6.380941806759	-6.070587832020
Si	-5.930943226102	-0.258854531367	-6.951950477381
C	-7.600227214868	-1.177555559227	-7.010649697075
C	-4.854838246091	-0.992168854739	-8.314059248876
C	-5.327707068793	-0.399477782059	-5.171603967384
H	-8.302239267559	-0.848313524282	-6.235786158672
H	-8.099843469881	-1.100325629271	-7.983799177711
H	-7.404348366588	-2.243379850704	-6.832233672100
H	-5.001863204252	-0.471953027978	-9.266729890137
H	-5.128883719237	-2.045323681080	-8.466895032314
H	-3.796152879557	-0.929219472633	-8.054809647454
H	-5.512570998965	-1.424489529193	-4.819551707711
H	-4.263363529202	-0.171066073592	-5.096895463252
H	-5.873249438867	0.275581954859	-4.502901336159
C	-2.152271407946	1.069415282269	-6.862091122628
H	-1.937235623042	1.657766233915	-4.807831550899
C	-1.370310961636	1.781726249486	-5.742076695231
C	-1.448162441111	1.054946414669	-8.242315609358
H	-2.264889373825	0.013094944158	-6.550361490577
H	-1.348271366160	2.865668208070	-5.926689712833
C	0.096546041864	1.316709506654	-5.461716604426
C	-0.198909151249	0.130303509221	-8.388178175134
H	-1.165437195529	2.080847895268	-8.520375692380
H	-2.173452207583	0.739523649387	-9.007249546760
C	1.147142440861	2.051409338917	-6.262139295169
H	0.164471115839	0.232507500118	-5.603894862214
H	0.316808207168	1.492552964966	-4.399832269255
C	1.140942546534	0.863067398963	-8.565282140280
H	-0.146344791964	-0.554845057641	-7.534672852542

H	-0.322482728780	-0.514200333527	-9.270411463115
C	1.563411503155	1.869303374622	-7.522273104128
H	1.115161898363	1.392265212984	-9.531115330861
H	2.336326431814	2.554732353578	-7.876606118647
H	1.607655090961	2.886000048988	-5.729885056023
H	1.944501959811	0.116178314936	-8.679798036618

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C1$_2$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.1161385245	0.2613664382	-0.0137114773
S	-3.0309792785	0.0407993179	-0.5906235054
C	-1.5621282661	1.1229111865	-0.2750810533
C	-4.3785219536	0.5764806133	0.5457095769
C	-1.0308740789	1.2623240412	1.0989391104
C	-1.5976740311	2.2954916014	-1.1315538828
H	-4.0485050212	0.5162442018	1.5845541657
H	-4.6017574188	1.6137729044	0.2885495916
H	-5.260542826	-0.0467708041	0.3803240561
C	-0.6465308657	2.5957509435	1.5171122539
H	-1.43144538	0.634743618	1.8995422412
C	-1.0994411555	3.4937319646	-0.6989196704
H	-1.9927322131	2.1987061264	-2.1411695234
C	-0.6377431328	3.6519518146	0.6496761903
H	-0.3588629849	2.7441064276	2.5562038588
H	-1.0703659798	4.3416826214	-1.3782692336
H	-0.314205629	4.6335314031	0.986177837
Si	-2.55006568	-2.087632305	0.0014758444
C	-4.2311285199	-2.938789298	-0.1279171663
C	-1.3628102313	-2.6481888498	-1.3374199242
C	-1.8365030099	-2.2171723135	1.7312594624
H	-4.9329510381	-2.6082095103	0.645785219
H	-4.6984184102	-2.7891700257	-1.1074205648
H	-4.086722571	-4.0187132334	0.0062291149
H	-1.8003566073	-2.5812284122	-2.3392203387
H	-1.0673459624	-3.689807651	-1.1586678501
H	-0.4589466413	-2.0302869254	-1.3000016296
H	-1.7288435039	-3.2793904262	1.9893301427
H	-0.8469517831	-1.7501501216	1.7568126712
H	-2.4707230514	-1.7523015948	2.4940441719
C	1.8969609872	-0.5191639418	0.2641549427
H	2.1430264415	0.3111819629	2.2252953759
C	2.6902304963	0.3313952163	1.271908848
C	2.5695346672	-0.6842853701	-1.1236630414
H	1.8214932125	-1.5359944432	0.6968647917
H	2.6929897005	1.3860632178	0.9611840192
C	4.1688234682	-0.0804675758	1.5741047919
C	3.8304151378	-1.6019071014	-1.1937093449
H	2.8278689668	0.3053854994	-1.5286107371
H	1.8343674942	-1.0995869057	-1.8317387826
C	5.1925527115	0.567871656	0.6710822125
H	4.2489573904	-1.1731816586	1.5568314331
H	4.4093987534	0.2198539524	2.6033851968
C	5.1546755247	-0.8756647896	-1.4816472947
H	3.9101805268	-2.1853213458	-0.2696774467
H	3.7004671449	-2.3437673739	-1.9951229077
C	5.5839736139	0.2481207113	-0.5695355858
H	5.1007172487	-0.4599093276	-2.5004988967
H	6.3388757898	0.898011466	-1.0176260447

H	5.6526566884	1.4637904297	1.0927724603
H	5.9672567361	-1.6203180311	-1.5291186782

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TS_{C1b} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.102368158103	0.068333455918	-0.337816538680
S	-3.352147440992	0.163671629563	-0.435843837913
C	-1.727200973359	1.064509794356	-0.401786240380
C	-4.448937804838	0.885042549132	0.862497889010
C	-0.992835153071	1.172661470955	0.894700110512
C	-1.805661025845	2.252503697086	-1.246088521166
H	-3.973519620089	0.817236382330	1.843010039808
H	-4.587190896528	1.933899814468	0.592553174671
H	-5.411802806692	0.368587736944	0.858434885838
C	-0.493241014798	2.489661862934	1.255252379805
H	-1.343118600888	0.588986738822	1.750172197686
C	-1.191909461459	3.415988918707	-0.884491727616
H	-2.330839316090	2.183937228401	-2.197641967923
C	-0.549214030502	3.547588017059	0.397306556020
H	-0.067746425763	2.618650043490	2.249198433329
H	-1.199989345083	4.263078896327	-1.566186885950
H	-0.141172952390	4.512643470330	0.686755528429
Si	-3.035360079629	-1.975672033066	0.197186594666
C	-4.794526746207	-2.634334770382	0.389697919265
C	-2.152866412143	-2.739374922187	-1.272203348061
C	-2.049542287805	-2.128642177230	1.786477591735
H	-5.319905754357	-2.189228209610	1.241793483235
H	-5.397160433534	-2.474095886994	-0.511028895577
H	-4.747525799352	-3.716576588387	0.567109543971
H	-2.727668611395	-2.645753857736	-2.199619692590
H	-1.975102990998	-3.805676982192	-1.083890799808
H	-1.180616121785	-2.256338615672	-1.410953481650
H	-1.991877622660	-3.189311841805	2.065772942061
H	-1.032987778405	-1.753596879948	1.627339199181
H	-2.499173507119	-1.586911446170	2.625609392105
C	1.621677403384	-0.763296860089	-0.241639638449
H	2.752360642202	-0.121985578503	1.454581741071
C	2.872565141362	-0.137080826217	0.362073244383
C	1.632129742460	-0.880025261563	-1.786235112150
H	1.538527820826	-1.788185576467	0.168679296097
H	2.968588299846	0.914871577846	0.057725206887
C	4.216557521634	-0.869854699292	0.039014451212
C	2.426537701590	-2.079357673313	-2.385693624302
H	2.011249858019	0.053618559301	-2.221675606543
H	0.583475732070	-0.953269854695	-2.167812192232
C	4.899014183600	-0.411670049565	-1.230487597164
H	4.030707431531	-1.950676701222	0.023591557285
H	4.921527919927	-0.698440181106	0.863978966414
C	3.686843247491	-1.666705916818	-3.165938109421
H	2.690492828465	-2.771478039439	-1.578335466342
H	1.794395121089	-2.654743594624	-3.076930947246
C	4.684314895523	-0.735455003832	-2.513617399059
H	3.363581361316	-1.178280363330	-4.098558265225
H	5.331071057401	-0.240614069274	-3.241331467442
H	5.681971750758	0.331080207332	-1.065431733391
H	4.213965150469	-2.576884360406	-3.497138198363

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C1$_3$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.6613419345	1.4404592956	0.112678838
C	0.7432041018	2.5362615865	0.6447542718
C	0.8377222043	2.5687839481	-0.7371217688
C	1.6561874537	3.2791805337	1.3898339295
C	1.7904064815	3.3055892867	-1.4390760878
H	0.0947747044	1.9616917587	-1.364358949
C	2.6321654385	4.0313788775	0.7207947499
H	1.6252049718	3.2877027635	2.4779150093
C	2.7005463133	4.0465339376	-0.6774183413
H	1.8352433462	3.3105017085	-2.5253124954
H	3.3490081888	4.6153303511	1.2946060376
H	3.464455136	4.6372105749	-1.1762468813
C	-2.0218520608	0.3157205463	-0.6283653476
H	-2.7980539402	0.9308167476	-2.546508944
C	-3.1642090296	0.7614359106	-1.5246114715
C	-2.2478846441	0.3488202956	0.8368373306
H	-1.5899670024	-0.6310084138	-0.9791317579
H	-3.5754465	1.719693372	-1.1778774035
C	-4.3133503361	-0.2903792599	-1.5951143561
C	-2.3192932053	-0.9938393286	1.5811698704
H	-3.105618365	0.9725552828	1.0999036715
H	-1.3518961538	0.9402048975	1.4307371169
C	-5.1022315567	-0.4519975118	-0.3120493843
H	-3.8713075163	-1.2508214537	-1.8941188935
H	-5.0027968987	-0.0053986337	-2.4000742562
C	-3.4373334948	-1.879837553	0.9716590022
H	-1.3622987499	-1.5237438505	1.5036922443
H	-2.5047952709	-0.8206080838	2.6493929193
C	-4.741884589	-1.141268145	0.7807362506
H	-3.5874732634	-2.7531510134	1.6190378383
H	-5.4187220292	-1.1332531211	1.6358326411
H	-6.0574397159	0.0729751435	-0.2795152908
H	-3.0833800836	-2.2592064499	0.0061229076

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C2$_1$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0568873558	0.2928739256	-0.1180613792
S	-2.5853122212	-0.5692699345	-1.6367312546
C	-1.6018377955	-0.8844353412	-0.1292999286
C	-3.5395047145	-2.1316151194	-1.7964164001
C	-0.4848780832	-1.9303783708	-0.3233993196
C	-2.408431476	-1.0218538552	1.0902118482
H	-4.1460082302	-2.3084558924	-0.9040011448
H	-4.1984149408	-2.0122107234	-2.6615800289
H	-2.8840333721	-2.9912632559	-1.9680336947
C	-0.335498723	-2.9490088156	0.7696453849
H	-0.5561990369	-2.4155312765	-1.3063524813
C	-2.1666478886	-1.9518762548	2.0451243042
H	-3.2306124973	-0.3209933355	1.2092984507
C	-1.1119891454	-2.9358554518	1.8697462158
H	0.4096576942	-3.7288149264	0.6248851829
H	-2.7758364697	-1.9866889641	2.9441786602
H	-0.9799186891	-3.6991721722	2.6334206398
Si	-1.1041774334	2.1942973978	0.5321622977
H	0.5186034022	-1.3970994428	-0.4284317193
C	-2.8897720556	2.5513035379	-0.0245992231

C	-1.0951052415	2.1946486373	2.4446172354
C	-0.1332337405	3.7521044521	-0.0213137641
H	-3.2082129434	3.5188814085	0.3885845259
H	-2.9678660049	2.6112789172	-1.1155987307
H	-3.6040534518	1.7918784165	0.3070372972
H	-1.6179391282	1.3203962716	2.8492140324
H	-1.5959921278	3.0935039525	2.8292683364
H	-0.0760182969	2.1849195038	2.8504466583
H	-0.5996303089	4.642996036	0.4209907215
H	0.9193227022	3.7523066619	0.2861717123
H	-0.1639026791	3.8797991277	-1.1105744997
C	1.7149218136	0.9559588146	-0.9189668791
C	1.8411412722	0.8259033105	0.4583588782
C	2.2340721576	0.0606790084	-2.0355918694
H	1.4787722103	1.9593565894	-1.2692809396
C	2.5155901514	-0.2712107771	1.2607827107
H	1.734743971	1.7496774109	1.026408165
C	3.2465644175	-1.0449265853	-1.6627618905
H	2.7162790495	0.7261012293	-2.7652266496
H	1.3914650836	-0.3914925303	-2.5805173736
C	4.0399945252	-0.06708519	1.384130994
H	2.3051845631	-1.2687226693	0.8707233586
H	2.0919784434	-0.2589514893	2.2727790454
C	4.5549069632	-0.5095398102	-1.1191642615
H	2.7909265079	-1.7668570426	-0.9794301414
H	3.4607111272	-1.608146814	-2.5793438918
C	4.864230974	-0.1076669512	0.1203796275
H	4.2240492895	0.9016202687	1.8724419697
H	4.4351395905	-0.8173532153	2.0874589001
H	5.3458210634	-0.4179749383	-1.8641322986
H	5.8845390784	0.2500332673	0.268345611

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TS_{C2a} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.3075652781	-0.7022797771	-0.4628560655
S	-2.4181806866	0.1643428377	-1.1453509452
C	-1.6967920418	-1.0038117151	-0.0130549339
C	-4.1902599616	-0.3984317712	-1.4739069403
C	-1.0292651894	-2.1595390621	-0.5903137274
C	-2.2233953561	-1.1188869964	1.3297463356
H	-4.7664987049	-0.3972441462	-0.5465385286
H	-4.6232982749	0.2999937144	-2.1951987759
H	-4.1606236154	-1.4045142397	-1.9008643007
C	-0.9326799311	-3.3599913803	0.2134848542
H	-1.0854570401	-2.3026739247	-1.6704413359
C	-2.0543928628	-2.2591756183	2.0611463292
H	-2.7844278051	-0.2881231849	1.7497227851
C	-1.3958579266	-3.4035542221	1.494242133
H	-0.4772080783	-4.2378016289	-0.2381319582
H	-2.4530806507	-2.3155377373	3.070726291
H	-1.3022835431	-4.3113455639	2.0839197474
Si	-1.5548314164	1.9780146341	0.294683443
H	1.2014052009	-1.8430575715	-0.8023950326
C	-3.2944911274	2.6974625392	0.5978381744
C	-0.7938226938	1.9959159227	2.040222704
C	-0.7274602947	3.1429520163	-0.949105322
H	-3.2054018648	3.672574043	1.0958806568
H	-3.8473095416	2.8466557556	-0.3369453397

H	-3.9050413434	2.0564267187	1.2457777063
H	-1.219746058	1.1980128223	2.6567265466
H	-1.0529591205	2.9530420558	2.5152002077
H	0.2904858093	1.8826968734	2.0578592563
H	-0.772204712	4.168446905	-0.5573417423
H	0.3184304836	2.9110296981	-1.1636962721
H	-1.2796899347	3.1273732911	-1.8953201323
C	1.7774412126	0.3507098071	-1.3278174705
C	1.7030063919	0.7107841901	0.0266218417
C	2.8839272176	-0.3396483375	-2.1134613293
H	1.2162211457	1.0192241227	-1.9895183746
C	2.5406920018	0.1647681735	1.1653694159
H	1.2401721313	1.6673621645	0.2461781693
C	4.0279222636	-1.0100183812	-1.3287607756
H	3.3275207181	0.4319825558	-2.7632094394
H	2.4290897494	-1.0750314222	-2.7873012823
C	3.8837898491	0.8872724274	1.3875374972
H	2.7020211046	-0.908538327	1.0438654219
H	1.9584906823	0.270615011	2.0909485703
C	5.0255376306	-0.0237854977	-0.7556497187
H	3.6071167187	-1.6773774819	-0.5716844276
H	4.5676349802	-1.6603445196	-2.0279896429
C	4.952184062	0.7532430502	0.3326488418
H	3.6874495544	1.9609692155	1.5354377074
H	4.3049279303	0.5452432961	2.3470102793
H	5.9289800571	0.0917675342	-1.3562529385
H	5.8099686027	1.4036351314	0.5157418364

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$C2_2$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.4159977567	-0.9111396431	-0.996418849
S	-2.4750578059	0.4013117401	-0.4226464607
C	-1.1383783978	-0.8491273305	0.1139719779
C	-3.991771389	-0.0742812845	0.5098755155
C	-1.153843873	-2.0064045508	-0.815857806
C	-1.1467619825	-1.1188120674	1.5443667119
H	-3.8216263602	-0.0207532253	1.5866554076
H	-4.8222410473	0.5676387516	0.2101536216
H	-4.1990682122	-1.1083480888	0.2276194945
C	-1.1593866749	-3.3288223575	-0.2246136248
H	-1.6939500796	-1.9207306208	-1.7595045095
C	-1.0595107708	-2.3967350346	2.0150245668
H	-1.1620052905	-0.2848193586	2.2430521252
C	-1.0752309916	-3.5244239473	1.1226577644
H	-1.2479293166	-4.18198772	-0.8946978666
H	-0.9813488896	-2.5676605011	3.0866144077
H	-1.0585471349	-4.5291620585	1.53615426
Si	-2.0859082639	2.5341963694	0.1885921745
H	0.8936624921	-1.8479794852	-2.0711280054
C	-3.8027724233	3.298788353	0.3706487744
C	-1.1281931878	2.6393068495	1.8010420934
C	-1.1864438446	3.2750323741	-1.2854185774
H	-3.6873554753	4.3773535068	0.540014759
H	-4.4114819115	3.1735783115	-0.5316791889
H	-4.3575734897	2.8923638928	1.2228584133
H	-1.6855881522	2.2039236036	2.6375073369
H	-0.9448849346	3.6954343562	2.0389277343
H	-0.1601088698	2.1360958821	1.7325212022

H	-0.9150685549	4.3161739092	-1.0685876462
H	-0.2681671121	2.7329146754	-1.5280912212
H	-1.8279958774	3.2718452566	-2.173444085
C	2.0597301621	0.0680972206	-1.5076566138
C	1.5473991428	0.5653445985	-0.2840813477
C	3.3744911286	-0.6483153308	-1.8003872262
H	1.7684857552	0.6644415118	-2.3780955836
C	2.0553765256	0.262407842	1.1166173633
H	1.0472653119	1.5350360327	-0.3411728133
C	4.1628173519	-1.2545996952	-0.6189494422
H	4.0379027068	0.0803845336	-2.293480716
H	3.1797803854	-1.4335959729	-2.5375837111
C	3.2803160069	1.0758603192	1.5735376198
H	2.2563969981	-0.8037067083	1.2497613424
H	1.2415856207	0.4737450981	1.8234385599
C	4.9925027573	-0.2326833337	0.1334869876
H	3.4849712442	-1.8137010473	0.0329309661
H	4.8541233888	-2.0002042502	-1.0304124087
C	4.6258976496	0.7276840158	0.991870689
H	3.0910336939	2.1461881365	1.3871036448
H	3.363142299	0.9937423058	2.6704890397
H	6.0542617301	-0.2557684245	-0.1174503474
H	5.4269182059	1.3723815905	1.360774497

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TS_{C2b} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.7482032725	0.858640014	-0.9359996464
S	2.4363318042	0.3389316609	-0.6055360213
C	0.8382879307	1.1792571232	0.0695524773
C	3.8236481239	1.1913853566	0.2551029896
C	0.49323793	2.3250036009	-0.806429049
C	0.8845093388	1.4052750522	1.5055566181
H	3.7430080956	1.073628721	1.3372547883
H	4.7766091008	0.8065033346	-0.1126985491
H	3.724839052	2.2480806751	-0.0009913162
C	0.2103831472	3.5902656995	-0.1624019656
H	0.9588741755	2.4012768733	-1.7896478042
C	0.5136902889	2.6074873417	2.0359385175
H	1.1580207219	0.584455085	2.165345099
C	0.1799928332	3.7244440959	1.1951482037
H	0.0333917379	4.4547405422	-0.7996888656
H	0.471952473	2.7244632587	3.1168323224
H	-0.0576209379	4.6812950501	1.6519715241
Si	2.6861127704	-1.8297691976	-0.0572706896
H	-1.5444034555	1.6635054993	-1.9255378812
C	4.5537675095	-2.1041411385	-0.0115824186
C	1.9072994257	-2.2261811482	1.6058181804
C	1.916001331	-2.7577072424	-1.4985270243
H	4.7456719543	-3.1765940018	0.1238405583
H	5.0410890905	-1.8004318547	-0.9446681672
H	5.0368514879	-1.5789498043	0.8191379356
H	2.0366574828	-3.29619264	1.8153378339
H	0.8360201815	-2.0079556478	1.6149060897
H	2.3799187959	-1.6698292902	2.4225580544
H	1.9561089232	-3.837789172	-1.3076325628
H	0.8688905635	-2.4844971228	-1.6572226312
H	2.4635579507	-2.5587698279	-2.4262951175
C	-2.1017212842	-0.5145463031	-1.3926198581

C	-1.3837869708	-0.8931567841	-0.231984172
C	-3.5791816573	-0.1752591287	-1.5636004524
H	-1.7256927544	-0.9779103458	-2.3101276759
C	-1.8483743404	-0.7892291809	1.211956776
H	-0.6432227712	-1.6841491194	-0.371915655
C	-4.4110192188	0.153213393	-0.3046497737
H	-4.0559247619	-1.0408662036	-2.0510912757
H	-3.6597893627	0.6571482835	-2.2696994125
C	-2.7701274866	-1.9219558126	1.7000738142
H	-2.3196755745	0.1759651018	1.4144169569
H	-0.9570879304	-0.7946823827	1.8537916998
C	-4.8754773636	-1.0808086987	0.4439548392
H	-3.8623626638	0.8540568509	0.3316175544
H	-5.3066295402	0.695208343	-0.6320836468
C	-4.1998400496	-1.9337055081	1.2247355996
H	-2.313790328	-2.8926462824	1.4437958125
H	-2.788708587	-1.9044669085	2.8028928216
H	-5.9201543886	-1.3391157668	0.2630159989
H	-4.7673710203	-2.7842908925	1.6091181661

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$C2_3$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.1448044988	1.0994452344	-0.7942476674
C	-0.1780307908	1.7416720886	0.6381144689
C	0.1365420125	2.6897197181	-0.3205966142
C	0.3796821768	1.832988756	1.9073865723
C	1.001717217	3.7550001492	-0.0743223359
H	-0.316429913	2.6083315942	-1.356396714
C	1.2516825433	2.8963448037	2.184171157
H	0.1570075802	1.1014840602	2.6817811311
C	1.5594398446	3.8478621637	1.2060024768
H	1.2368840872	4.4894624783	-0.8402501178
H	1.6977113967	2.9824313135	3.1726236213
H	2.237618542	4.6642639583	1.439187741
H	-1.6103317701	1.0864648227	-2.2157158854
C	-2.3756831116	-0.4229133186	-1.1503477219
C	-1.8632123903	-0.4524550008	0.1701536281
C	-3.821884014	-0.0811412728	-1.5210919842
H	-1.8999735784	-1.105856188	-1.8510922946
C	-2.7216035723	-0.243148149	1.4000895619
H	-1.0252851266	-1.1304940056	0.3401911158
C	-4.9264868941	-0.8233757047	-0.7043904338
H	-3.9400562938	-0.3070409522	-2.5868055235
H	-4.0088676846	0.9925933631	-1.4264344658
C	-3.3110516222	-1.5907871883	1.9030788665
H	-3.5168243269	0.4788788899	1.1963409312
H	-2.1277760145	0.1866933584	2.2140116762
C	-4.5789355526	-2.2178576331	-0.24507443
H	-5.1915321248	-0.2159396089	0.1668745352
H	-5.8303752239	-0.8594633902	-1.3248102054
C	-3.9046446809	-2.5287951933	0.8691637077
H	-2.507246329	-2.1366690598	2.4150576514
H	-4.0555974123	-1.3762826285	2.6860771845
H	-4.9086013327	-3.0375818937	-0.8834466448
H	-3.7488601424	-3.587657565	1.0775460119

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C3$_1$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.1448044988	1.0994452344	-0.7942476674
C	-0.1780307908	1.7416720886	0.6381144689
C	0.1365420125	2.6897197181	-0.3205966142
C	0.3796821768	1.832988756	1.9073865723
C	1.001717217	3.7550001492	-0.0743223359
H	-0.316429913	2.6083315942	-1.356396714
C	1.2516825433	2.8963448037	2.184171157
H	0.1570075802	1.1014840602	2.6817811311
C	1.5594398446	3.8478621637	1.2060024768
H	1.2368840872	4.4894624783	-0.8402501178
H	1.6977113967	2.9824313135	3.1726236213
H	2.237618542	4.6642639583	1.439187741
H	-1.6103317701	1.0864648227	-2.2157158854
C	-2.3756831116	-0.4229133186	-1.1503477219
C	-1.8632123903	-0.4524550008	0.1701536281
C	-3.821884014	-0.0811412728	-1.5210919842
H	-1.8999735784	-1.105856188	-1.8510922946
C	-2.7216035723	-0.243148149	1.4000895619
H	-1.0252851266	-1.1304940056	0.3401911158
C	-4.9264868941	-0.8233757047	-0.7043904338
H	-3.9400562938	-0.3070409522	-2.5868055235
H	-4.0088676846	0.9925933631	-1.4264344658
C	-3.3110516222	-1.5907871883	1.9030788665
H	-3.5168243269	0.4788788899	1.1963409312
H	-2.1277760145	0.1866933584	2.2140116762
C	-4.5789355526	-2.2178576331	-0.24507443
H	-5.1915321248	-0.2159396089	0.1668745352
H	-5.8303752239	-0.8594633902	-1.3248102054
C	-3.9046446809	-2.5287951933	0.8691637077
H	-2.507246329	-2.1366690598	2.4150576514
H	-4.0555974123	-1.3762826285	2.6860771845
H	-4.9086013327	-3.0375818937	-0.8834466448
H	-3.7488601424	-3.587657565	1.0775460119

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TS$_{C3}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.343225118	0.4936718117	0.5221184286
S	-1.5842786981	0.0080906004	-0.5633683201
C	-0.9662004678	1.817571653	-1.0348206252
C	-1.5012862786	-0.8795109092	-2.1574974309
C	-1.9721940769	2.8431329393	-0.899594996
C	-0.0858718171	1.9355638033	-2.1629852715
H	-1.3622172191	-0.1403225796	-2.9534646739
H	-0.6855907039	-1.6022835239	-2.1738292293
H	-2.4556064023	-1.3935561648	-2.2927545457
C	-1.9874743659	3.9398350956	-1.7403759948
H	-2.711726011	2.748112508	-0.1099507935
C	-0.1404953837	3.0499777678	-2.9957493433
H	0.659915988	1.1671439971	-2.3429341684
C	-1.0735725799	4.0691635446	-2.8000855437
H	-2.749116119	4.7013290336	-1.5870739152
H	0.5655332621	3.1130746708	-3.821120611
H	-1.1081230731	4.9285796081	-3.4616248266
Si	1.2900643442	-1.6131403111	0.4489076497
H	-0.2905278509	1.8733882531	0.1127705962
C	-0.0306437345	-2.9950809073	0.5716016899
C	2.1603044464	-1.7447522607	-1.2601108159

C	2.6387441567	-2.2138536174	1.6671225621
H	0.4204960358	-3.9747470142	0.3623832594
H	-0.4406180527	-3.0351403296	1.5887770302
H	-0.8766311455	-2.8662910012	-0.1119697421
H	1.5255791226	-1.4718393232	-2.1112087086
H	2.5160738991	-2.7707179827	-1.4284468906
H	3.0379146873	-1.0861180798	-1.2892277606
H	3.0248640735	-3.1825382773	1.3211656897
H	3.4950301835	-1.5326764491	1.7394256657
H	2.2435417912	-2.3668477491	2.6777217161
C	1.7560011383	0.9820307292	1.8782666871
C	1.2048881898	2.1451583035	1.2962396975
C	1.5070949036	0.5353893646	3.3220134387
H	2.7335999534	0.695828853	1.4963793437
C	0.3891539114	3.1796346962	2.0489422837
H	1.7726161111	2.5735093359	0.4644755264
C	1.6174441421	1.6418192712	4.4203126481
H	2.2349990991	-0.2487599184	3.5457798272
H	0.5226124026	0.0657590473	3.4335295852
C	1.3021999779	4.2673964759	2.6770800103
H	-0.2305201323	2.7001599267	2.8108717857
H	-0.3052014983	3.6888276419	1.3676258508
C	2.6716774027	2.6933468463	4.1801721113
H	0.6443182827	2.1253296381	4.5477786873
H	1.8206790167	1.1363359458	5.3726127677
C	2.5217186206	3.8044987346	3.4487810464
H	1.654124332	4.9161022711	1.8637283518
H	0.6799233928	4.9173273419	3.3127507617
H	3.6431148762	2.5206100218	4.6434796129
H	3.3761239694	4.4789922972	3.3855461864

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$C3_2$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.0442140441	-1.0198470788	0.7686640652
S	-1.921117508	-1.8388037992	0.7923397726
C	-2.8019885832	-1.6473510755	-0.8172285773
H	-3.5329908105	-0.8397284811	-0.7257179088
H	-2.1200939733	-1.4117944985	-1.6364547211
H	-3.3281721809	-2.5760804165	-1.0527721593
Si	1.0325864868	-2.6500320473	-0.3776870014
C	0.0197820071	-3.4692044052	-1.7583887394
C	2.5930148827	-1.981715766	-1.2531153652
C	1.5566313594	-3.9970182424	0.8578139346
H	0.6505025871	-4.2005408895	-2.2827551174
H	-0.8547597368	-3.9902681506	-1.3582384994
H	-0.32639209	-2.7462829336	-2.50603439
H	2.3350419183	-1.2458257541	-2.024288051
H	3.0973372287	-2.8169357945	-1.7586374287
H	3.322060941	-1.5198908469	-0.5783061116
H	2.1105233474	-4.7867477036	0.3317711285
H	2.2049431153	-3.6096119208	1.6517689965
H	0.6809970067	-4.4555232365	1.329558685
C	1.6892565121	-0.4009069309	1.7518984269
C	1.2762600521	0.5259442724	0.7900729566
C	1.4030486981	-0.4555146676	3.2467033195
H	2.5571303024	-0.9979261804	1.4768580556
C	0.3886890992	1.7470750375	0.9679302922
H	1.8790227537	0.5594870897	-0.1183233308

C	0.7001660878	0.7545832612	3.8989756285
H	2.3713622122	-0.5959796202	3.748102316
H	0.826890101	-1.364624623	3.4779978878
C	1.1334658308	2.9842768141	1.5115573008
H	-0.4803376683	1.5284070358	1.5933143079
H	-0.0184860054	2.0093594998	-0.0166692761
C	1.5357286463	2.0173301905	3.8823549995
H	-0.2852077045	0.9061555343	3.4509528956
H	0.5046582921	0.4875310543	4.9444816745
C	1.7143148978	2.9113654647	2.9017666179
H	1.9508687892	3.2303606357	0.8171936973
H	0.4499898872	3.8467957727	1.4613382576
H	2.0940320921	2.1971909542	4.8015777807
H	2.3820270821	3.7449634458	3.1258206804

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C4$_1$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.3225002657	-0.1814320468	0.7438277808
S	-1.3190475636	-1.4838794576	0.0384199704
C	-2.8011201415	-0.7610252134	-0.6853371722
C	-0.9024610493	-2.7167645171	-1.2485912739
C	-3.9763206959	-0.7582972657	0.0741261956
C	-2.7924271264	-0.1720542287	-1.9566621543
H	-1.7495206237	-3.3922242291	-1.3896044382
H	-0.6354364675	-2.2450336941	-2.196775023
H	-0.0438391896	-3.2776787757	-0.8735994699
C	-5.135442691	-0.1688746116	-0.4352428811
H	-3.9789117304	-1.2180122077	1.0578858205
C	-3.9572566593	0.4022291202	-2.4666203962
H	-1.8785132855	-0.1572637946	-2.5436144542
C	-5.129873333	0.408250429	-1.7062154154
H	-6.0443930532	-0.1682958194	0.1601894034
H	-3.9457160337	0.8544453743	-3.4547272762
H	-6.0336101446	0.8619874398	-2.1032817645
Si	-0.3821617774	2.114493585	0.9757394084
H	-0.6281696782	0.6847355233	1.6371493262
C	0.5230048419	3.1497478617	2.2750908865
C	0.2431644415	2.47081204	-0.7890354962
C	-2.1984837608	2.6643433429	0.9434510065
H	0.4388719885	4.218818453	2.0405360903
H	0.070691014	2.9917509663	3.2616217763
H	1.5847999712	2.9018652814	2.3520431152
H	1.2795110412	2.1771219462	-0.9731435563
H	0.159474168	3.5508704786	-0.9778069167
H	-0.3909153943	1.9637698084	-1.5249172364
H	-2.2761772775	3.7279265794	0.6824896373
H	-2.7661349384	2.0976098569	0.1973379312
H	-2.6911244869	2.5246809886	1.913043394
C	2.2169035485	-0.1523354037	1.2687439828
C	1.9262286082	-1.2016936279	0.3436214665
C	3.1929333439	1.0130395572	1.0513868592
H	2.2247404953	-0.4795472042	2.3122818835
C	2.4939420805	-1.283564858	-1.0630363913
H	1.8010600331	-2.196731555	0.7890883809
C	4.4585896739	0.7413892127	0.1836493832
H	3.5300845661	1.3353732232	2.0453010735
H	2.7069273489	1.8940640324	0.6160116183
C	3.8212062449	-2.0855135626	-1.1225989559

H	2.6255184961	-0.2833723893	-1.4857303981
H	1.7864912881	-1.7897751801	-1.7348528165
C	5.1642318349	-0.562358753	0.4559215214
H	4.1934302264	0.8017405446	-0.8761171069
H	5.1570416053	1.5709636731	0.3578909582
C	4.8937496368	-1.7452712609	-0.1083627522
H	3.5733020501	-3.1481005957	-0.9871318289
H	4.2362624452	-2.0183540622	-2.1420167361
H	5.9661673911	-0.5286783233	1.1943635161
H	5.5144024525	-2.591344681	0.1900225242

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TS_{C4} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0609131996	-0.166242833	0.3479980827
S	-1.3766406051	-2.1600648648	0.5294625483
C	-2.4801657874	-0.4809959282	0.02016928
C	-1.5162273221	-3.1333480982	-1.005468272
C	-3.5199075418	-0.2335835799	0.9756906076
C	-2.8342418394	-0.3636527094	-1.3579861757
H	-2.4579202647	-2.8765561031	-1.5026564065
H	-0.6830403847	-2.9600541643	-1.69260074
H	-1.5317486804	-4.1877339895	-0.7185088508
C	-4.7905398584	0.132402583	0.5685562089
H	-3.29704617	-0.3429769092	2.0329217571
C	-4.1266679271	-0.0016429146	-1.7361887307
H	-2.0772345725	-0.5142443843	-2.1219058922
C	-5.1205580772	0.2495167124	-0.7910772384
H	-5.5484547467	0.3118695709	1.32779292
H	-4.3491128768	0.0898221179	-2.7971741947
H	-6.1229515798	0.5308515183	-1.097311957
Si	-0.045910613	2.1236046876	0.322167197
H	-1.5085964076	0.3748160523	0.3057679185
C	-1.1757695817	2.7959186918	1.7101235813
C	1.6009097057	3.0706400099	0.5620788065
C	-0.7239345208	2.7276872785	-1.3584007104
H	-1.2547780413	3.8902465882	1.6556396388
H	-2.190533081	2.38463266	1.6494081223
H	-0.7751091888	2.5444372602	2.7006036547
H	2.0852102368	2.8580105838	1.5213928984
H	1.375476832	4.1462142905	0.5467026025
H	2.3296612612	2.8866159745	-0.2352426327
H	-0.839223863	3.8200641802	-1.3570411532
H	-0.0396389601	2.4699716657	-2.1767638775
H	-1.7012098142	2.2890996828	-1.590685779
C	1.7471673465	-0.9259471232	1.0579596002
C	1.7105334499	-0.9620470697	-0.3273384763
C	2.6498262734	-0.1176376413	1.9761035267
H	1.3182869654	-1.7966798671	1.5529746733
C	2.5479291197	-0.1571306322	-1.292718362
H	1.3137665173	-1.8803594393	-0.7668650778
C	3.9926744715	0.386468864	1.392447805
H	2.8763089409	-0.7690136469	2.8308444416
H	2.1074017809	0.7366032235	2.4011370406
C	3.8896212241	-0.8560139685	-1.6160004031
H	2.7183617362	0.8526752648	-0.9226453156
H	1.9963084261	-0.0432091586	-2.2353341805
C	4.8500959907	-0.6994250432	0.7818121585
H	3.8137321104	1.1925313326	0.6792371876

H	4.5482822011	0.8463485301	2.2195350858
C	4.8020626315	-1.1988381268	-0.4598835676
H	3.6695385606	-1.7916929975	-2.1505426662
H	4.4385594727	-0.237070051	-2.3434125995
H	5.5936514841	-1.1320365807	1.4518601995
H	5.5289067665	-1.9762654986	-0.6997592839

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$C4_2$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.6986941821	-0.7093491863	0.7789376024
S	0.9284973166	-1.9124880965	1.4371182985
C	1.3731165038	-0.5699247849	2.6311681287
H	2.1327767257	0.0966395277	2.2138898217
H	0.5060177407	0.02988741	2.938266804
H	1.7735781702	-1.0397206654	3.5341778164
Si	-0.5677530975	-1.8258920686	-1.1635750114
C	-0.0391905562	-3.6459452727	-1.0630418891
C	-2.2944613867	-1.9036605443	-1.972754283
C	0.613671878	-0.9012380087	-2.3281885924
H	-0.1301519894	-4.0986536324	-2.0601249549
H	0.9945727284	-3.7639781027	-0.7267918484
H	-0.6817998471	-4.2147039621	-0.381668998
H	-2.9937778218	-2.4965225682	-1.3723633495
H	-2.1815531704	-2.4173629212	-2.9380140822
H	-2.7551427731	-0.9326200414	-2.1734972483
H	0.6361343149	-1.4031601716	-3.3053743164
H	0.3130107707	0.1385518699	-2.494808064
H	1.6307083365	-0.9022181106	-1.9224564239
C	-2.37575493	0.2656557228	1.2253535591
C	-1.5084834812	1.0901221228	0.4952303268
C	-3.7716849409	-0.2266981687	0.8646111597
H	-2.2099487164	0.2783771574	2.309445026
C	-1.7562741279	1.7309163463	-0.8526374475
H	-0.8010889789	1.674269737	1.0973412481
C	-4.5778332442	0.6354947398	-0.1391036066
H	-4.3405941365	-0.2772501032	1.8018577837
H	-3.7417520008	-1.2566766583	0.487412379
C	-2.5063482284	3.0777915073	-0.7251760611
H	-2.286803809	1.0589259363	-1.5272948283
H	-0.7906852668	1.9367804373	-1.3319750071
C	-4.6953006434	2.0924744522	0.2450624485
H	-4.1589510868	0.5312236781	-1.1423554056
H	-5.5853335101	0.2044206272	-0.1969694958
C	-3.8367853115	3.0890549947	-0.0061329909
H	-1.8463718043	3.7860628871	-0.2031885664
H	-2.6348477769	3.5027778385	-1.7336098718
H	-5.591902007	2.3509953704	0.8092476309
H	-4.1230556602	4.0786257048	0.3532743089

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$N1_1$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.6067224775	0.3050266874	0.2586399303
S	1.5915795458	1.5688923264	-2.427116411
C	0.7437777758	1.6301317705	-0.8612273339
C	2.6448447759	0.0856553367	-2.25645973
C	-0.5478187148	2.2071171401	-0.8351482712
C	1.2938291951	1.1698429887	0.3637966597

H	2.0490566055	-0.7768614929	-1.9453126158
H	3.0571709344	-0.1025828626	-3.2511676655
H	3.4725392964	0.246260642	-1.5608907848
C	-1.2319861112	2.4090423535	0.3866888221
H	-1.0237497128	2.4907539145	-1.7677924135
C	0.5979695105	1.3631790745	1.586113027
H	2.2640012676	0.6877807187	0.384681631
C	-0.6550562056	2.0155161804	1.6082392635
H	-2.2241961659	2.8472152779	0.369269828
H	1.0444698415	1.0059115915	2.5077609746
H	-1.1806563947	2.169866656	2.5440078848
Si	-0.678604737	-1.8750613697	0.6417837028
H	-1.6807761356	-0.5879980978	-0.2335293521
C	0.9096262712	-2.2318076253	1.6604947735
C	-2.1019433352	-2.4775883187	1.7503973548
C	-0.5281318256	-3.0103610927	-0.8783358204
H	0.9656521115	-3.3035748115	1.8982658951
H	1.8225318819	-1.970506937	1.1116571724
H	0.9220106282	-1.6850494442	2.611038832
H	-2.1568245982	-1.8729015572	2.6646263205
H	-1.9515787235	-3.5216416489	2.0550133579
H	-3.0744124017	-2.4083343856	1.24952915
H	-0.3720082787	-4.0547196077	-0.5776120459
H	-1.4198079749	-2.9714257263	-1.5144801353
H	0.3294981517	-2.7172306806	-1.4980410004

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TS_{N1} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.180948968	0.5021072883	0.0681419997
S	2.5564647023	-0.1128341571	-0.9941430181
C	1.9336870801	1.2364579153	0.0151158466
C	4.4177594612	-0.0563799298	-0.8854777681
C	0.9811352105	2.1084531766	-0.6535426239
C	2.5822887631	1.6543990679	1.2230719734
H	4.7709825128	-0.2201672286	0.1337741658
H	4.8029701036	-0.8361490413	-1.5455373381
H	4.7297240345	0.9279639588	-1.2422892359
C	0.6535267723	3.3302036778	0.0206235755
H	0.8659744117	2.0855634356	-1.737717702
C	2.2106176154	2.8361790911	1.8200748981
H	3.3498308364	1.0316426238	1.6752400323
C	1.2221441626	3.6698315618	1.227942239
H	-0.0383589318	4.0170861521	-0.4617561369
H	2.6812827548	3.1390049412	2.7516595652
H	0.9483768704	4.6014809405	1.715231183
Si	1.5775714233	-1.9659453124	0.084845353
H	-0.9269810561	-0.507255968	0.3903622025
C	3.145354673	-3.0543176007	-0.0680387213
C	1.2569762112	-1.8753496389	1.9475550234
C	0.3161492864	-2.7842453888	-1.0569076776
H	2.8981703554	-4.0583320482	0.3034624462
H	3.4898935199	-3.1724840933	-1.1031052011
H	3.9877839388	-2.6894893261	0.5319039722
H	1.7279823542	-0.9955618238	2.3972934484
H	1.6662679436	-2.7686531729	2.4398252149
H	0.1835625958	-1.7986824148	2.132129084
H	0.5578870338	-3.8474312884	-1.1888945967
H	-0.6881400329	-2.6725289437	-0.6429084892

H	0.3175944256	-2.3121264543	-2.0452697141

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N1₂ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.6041445293	0.559796528	0.1409310518
S	1.4749779583	-1.02449233	-1.1855511274
C	-0.2580272036	2.067106203	0.7136519343
C	3.3079259123	-1.1943776987	-1.0761800929
C	0.0324450232	3.1319534895	-0.1620250199
C	-1.2197614149	2.2944051262	1.7112064073
H	3.6329579327	-1.2980762487	-0.0392073273
H	3.6326187003	-2.0551191197	-1.6648412731
H	3.7403579847	-0.2870229655	-1.5019013209
C	-0.618398374	4.3654390136	-0.0611787897
H	0.7848142954	3.0099855416	-0.945384106
C	-1.8728729427	3.5251476581	1.8206700638
H	-1.46089965	1.5022518459	2.4160804176
C	-1.5762378596	4.5648368016	0.9346836713
H	-0.3750948542	5.1694934049	-0.7532513296
H	-2.6170116723	3.6752238446	2.6007601839
H	-2.0835131945	5.52259911	1.0235507658
Si	0.7043093021	-2.9022176147	-0.3096777499
H	0.7051200863	0.1516856547	1.511242634
C	1.2176509758	-4.3242954219	-1.4389527915
C	1.3976729193	-3.1221651596	1.4257654985
C	-1.1609503601	-2.6654229894	-0.2888177758
H	0.8214628327	-5.2707119706	-1.0487729903
H	0.8271639478	-4.1884730877	-2.4532732309
H	2.3066831573	-4.4290273343	-1.5048852951
H	2.4874022067	-3.2391896996	1.4296816062
H	0.9707969549	-4.0228274246	1.885876495
H	1.1432937732	-2.2614227646	2.0519956168
H	-1.6439788118	-3.5575103416	0.1299585606
H	-1.44024252	-1.8056257941	0.3287063418
H	-1.5640936348	-2.5083962564	-1.2953780284

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N2₁ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.1235917541	-0.3013828542	0.2452198666
C	0.9326909314	-2.1273668275	0.2352219168
C	0.9062302706	-1.5717080442	-1.0671629193
C	1.4422905887	-1.3632364723	1.3081728584
C	1.3795459738	-0.2597186811	-1.3044680133
H	0.4949162985	-2.1483108684	-1.8884561491
C	1.8936083401	-0.0489291623	1.0748819002
H	1.4693826382	-1.7732018729	2.3120996553
C	1.8703849873	0.5154934951	-0.2284689164
H	1.3467495055	0.1632127861	-2.3023736362
H	-1.0703825815	0.6637725631	0.8509827919
H	2.2558769674	0.5446638439	1.9068424051
Si	-2.3265890457	-0.3860131764	-0.0115273799
H	-3.3229742345	0.0691501115	2.2685605034
C	-3.1205729666	1.0604359239	-0.9567943767
C	-2.6007719405	-1.9101459931	-1.144308393
C	-3.3306372826	-0.7657452725	1.5583815067
H	-4.1617957164	0.8346067156	-1.221864586
H	-3.115109759	1.9902836736	-0.3762064814

H	-2.5771698106	1.2505418298	-1.8910862191
H	-2.131134807	-1.782047249	-2.1269072287
H	-3.6771177373	-2.0577935529	-1.3119437153
H	-2.2080726834	-2.8328488873	-0.7005504643
H	-4.3767214038	-0.9919676104	1.3134982669
H	-2.9165352167	-1.6419537561	2.0734265307
H	0.560056073	-3.131729992	0.4038132602
S	2.4894203554	2.1586605562	-0.5685011189
C	1.5855145	3.1548294079	0.6765028468
H	1.7478180406	4.2016988198	0.4061136144
H	0.5180456437	2.9246046017	0.6342526717
H	1.9656718256	2.9887659445	1.6876080028

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TS_{N2a} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.053896127	0.0899416982	0.2753894311
C	2.1200270291	-2.5052085325	0.1147907906
C	2.3892087432	-1.7447255091	-1.0727627365
C	1.6375745862	-1.9206084484	1.2482320177
C	2.2265188634	-0.3879903781	-1.1394948659
H	2.7393103003	-2.2685367499	-1.957292559
C	1.3735823404	-0.4796088285	1.3248000288
H	1.4386517509	-2.5079565111	2.140255372
C	1.756493457	0.4355725883	-0.023080513
H	2.4513425954	0.146841914	-2.057393694
H	1.3594239634	0.0019290298	2.305365041
H	2.4996596757	-0.0685254919	0.9684209769
Si	-2.3991753549	-0.0869441596	0.3019670082
H	-2.9014317893	1.0715635272	2.5011900841
C	-3.2507535819	1.2968642493	-0.7340428333
C	-3.1160373573	-1.7264910324	-0.393873738
C	-3.1673112169	0.1045525045	2.0544317411
H	-4.3451235012	1.2050477668	-0.6888726244
H	-2.9922236149	2.2981243295	-0.3643457252
H	-2.9616569308	1.2532914054	-1.792049912
H	-2.8180719209	-1.8758034749	-1.4396569882
H	-4.2144319797	-1.7366976149	-0.3571617799
H	-2.7580375015	-2.5954490116	0.1730154933
H	-4.2643304623	0.0478749753	2.0186874673
H	-2.8194048757	-0.6784035169	2.7405201594
H	2.301685457	-3.5755858385	0.1013732025
S	2.3239937898	2.1500861654	0.0391208788
C	0.7945569238	3.0621588454	0.4789269106
H	1.0815950107	4.1178833272	0.5008914216
H	0.0199752215	2.9107860499	-0.2734726738
H	0.4215285066	2.7682777219	1.4618276182

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$N2_{2a}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.3304337975	-0.8930598218	-0.0116398862
C	1.2894183174	-2.1940064167	-0.4258593524
C	1.7174481173	-1.3078460033	-1.5057380174
C	1.2329468964	-1.7015447171	0.8875040322
C	2.1184103707	-0.0345001878	-1.2776204827
H	1.7003817774	-1.6970956628	-2.5215848057
C	1.2184140199	-0.2680936346	1.0297502211
H	1.001594983	-2.3632064702	1.719660995

C	2.1994296488	0.4934508193	0.1382975442
H	2.4801019355	0.5912278599	-2.088737191
H	1.0981450631	0.1401200363	2.0292861115
H	3.2236146847	0.327068989	0.5217879506
Si	-2.1862233253	0.1101110648	0.3839549378
H	-3.0511943952	0.4873201537	2.7094360064
C	-2.91708366	1.6547527559	-0.4487291301
C	-2.2934951807	-1.3786796868	-0.8849333124
C	-3.2145051913	-0.2733832449	1.9363908095
H	-3.9970556471	1.5422914112	-0.612675051
H	-2.7743537745	2.5492292154	0.1694066756
H	-2.4443424299	1.843396469	-1.4189601699
H	-1.3433075193	-1.9353745522	-1.1137126107
H	-2.6376195383	-1.0118687826	-1.8555635496
H	-2.9681391318	-2.1588140465	-0.5216603941
H	-4.2894792434	-0.2917444674	1.7138469885
H	-2.9390891585	-1.2427587391	2.3668671883
H	1.1743238872	-3.2545010378	-0.6274291421
S	2.1428138287	2.3388398128	0.2613384836
C	0.6149079914	2.7982513378	-0.6228880936
H	0.591040229	3.8918464875	-0.6329377546
H	0.6255354376	2.4347055913	-1.6547379392
H	-0.2716951955	2.4216454675	-0.1127120616

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N2$_{2b}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.1687360841	-1.088023258	0.2592193463
C	1.6053670519	-2.0956295948	-0.3221982129
C	1.6909997528	-1.3085837042	-1.5526545488
C	1.6681357757	-1.4289333119	0.9105554377
C	1.8021705946	0.0391562111	-1.5434022019
H	1.6531030839	-1.8398765205	-2.5013087918
C	1.3464389296	-0.02802243	0.9083948043
H	1.743004674	-1.9857425357	1.8422522389
C	1.851272388	0.8216250557	-0.2503822781
H	1.8977663591	0.5879313552	-2.4764975772
H	1.3166658529	0.4835657597	1.8661759867
H	2.8790266741	1.1743536683	-0.0524036976
Si	-2.0581766366	-0.1531650296	0.6566788473
H	-2.7793041898	0.5680860816	2.9477627659
C	-2.8820934196	1.2139067912	-0.3665932058
C	-2.1386812702	-1.8525033087	-0.3125100146
C	-2.9584968813	-0.3152285985	2.3229054107
H	-3.9656904507	1.0589913558	-0.4542144156
H	-2.7209394196	2.1930143785	0.0987537148
H	-2.4534985789	1.259324508	-1.3731183481
H	-1.1584972885	-2.3805425264	-0.5030573203
H	-2.5670522994	-1.7134262575	-1.3083741445
H	-2.7207017671	-2.5914407747	0.244905076
H	-4.0442692039	-0.4086745679	2.1888526937
H	-2.6076517973	-1.1901921211	2.8817645155
H	1.7172911455	-3.1739369214	-0.3769552508
S	0.8434367987	2.3859934979	-0.337474249
C	2.058250018	3.5097251739	-1.1153447908
H	2.9541628746	3.6225806897	-0.4962970768
H	2.3461388981	3.1702724829	-2.1155085447
H	1.5720344153	4.4848034514	-1.2091071684

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TS_{N2b} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.6287740369	-0.3455628487	-0.2872516477
C	1.1054614193	-1.707678632	-0.6823096654
C	2.168916955	-0.9875565981	-1.3673652131
C	0.7948779116	-1.2980004842	0.6379737544
C	2.5337095018	0.2598283435	-0.9901941078
H	2.7129300111	-1.5053464829	-2.155547899
C	0.8808311073	0.0981734755	0.9144973078
H	0.4430463603	-1.9955524127	1.3945089222
C	1.6718663485	0.9995029689	-0.0326273464
H	3.3828220061	0.7695563982	-1.4345202311
H	0.7410940786	0.453946409	1.930463724
H	2.2047378041	1.7931229049	0.4950743564
Si	-2.5383505854	0.0806780051	0.5955263048
H	-3.1242860801	-0.6560257336	2.9232730062
C	-3.4522862933	1.7434472082	0.5879870748
C	-2.6291910673	-0.7548734008	-1.1609480429
C	-3.3237709418	-1.0405181254	1.9155355704
H	-4.5389656582	1.6160963715	0.4932545156
H	-3.266063443	2.2906578233	1.5200071102
H	-3.1015881079	2.3733424057	-0.2362732566
H	-1.6485855509	-0.9822330825	-1.6644221387
H	-3.1455209188	-0.0923555851	-1.8607668371
H	-3.1394546671	-1.7203561814	-1.113162588
H	-4.4140537029	-1.0987165176	1.7975288532
H	-2.9221450885	-2.0589786545	1.8651895415
H	0.9378557453	-2.7446697884	-0.9589949229
S	0.2465494652	1.9114456077	-1.0183599537
C	0.9809562825	2.3393494005	-2.6415197788
H	1.7263647237	3.1341089274	-2.544938357
H	1.4306619681	1.4601762043	-3.1085076871
H	0.1580249738	2.7006785742	-3.2646613482

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$N2_3$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.344367165	0.0091583891	0.0339057834
C	1.7087352341	-1.8034284335	-0.5108163331
C	2.6908276479	-0.8234304949	-0.6636716252
C	0.9455090654	-1.8499526513	0.6824722268
C	2.9654813403	0.0884354162	0.3805548554
H	3.2469045703	-0.7551100564	-1.5932219781
C	1.1981150651	-0.9080285656	1.7125735737
H	0.2141832153	-2.6353921379	0.8318888054
C	2.2400136792	0.0404543685	1.5682055318
H	3.725131912	0.8500634658	0.238716977
H	0.6483586612	-0.9688581029	2.6452472282
H	2.448242543	0.7419371677	2.3693688905
Si	-1.8474558049	0.0399304254	0.4276873883
H	-1.6912994647	-1.4039892385	2.5461673125
C	-2.4009145742	1.5903654625	1.3773633254
C	-2.9801536459	-0.2784216812	-1.0660099642
C	-2.2568354587	-1.4215126048	1.6069504842
H	-3.4611887608	1.5037216279	1.6518931704
H	-1.8308725919	1.7092937679	2.3071580128
H	-2.2705232355	2.4966058797	0.7793712443
H	-2.9940141768	0.5705581751	-1.7553774105

H	-4.0069782165	-0.4576226373	-0.7191356593
H	-2.6677755724	-1.1695639169	-1.6249138569
H	-3.3213505821	-1.3582016768	1.8730880075
H	-2.103822451	-2.4003224794	1.1361211924
H	1.5216991251	-2.5220063566	-1.3021365679
S	-0.1163270959	1.6994350617	-1.2358428443
C	-0.083698072	0.980180738	-2.930676311
H	-0.2377262672	1.800041687	-3.6385609042
H	0.87539588	0.5035542233	-3.1547643783
H	-0.8867121334	0.250488178	-3.0715501769

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T1$_1$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.29626522	0.4875323947	-0.1587845545
S	-3.3337874597	0.5918810492	0.6699244533
C	-2.0184950169	1.3894647226	-0.2986373178
C	-4.5356577367	1.9675202935	0.8435933667
C	-1.0287479359	2.2096071751	0.3990581037
C	-2.3494960581	1.7599284873	-1.6593734415
H	-4.0963762857	2.8004226967	1.399834411
H	-4.8692605857	2.3180709374	-0.136779381
H	-5.3940024125	1.5763613402	1.3981067752
C	-0.5121003735	3.3803285085	-0.2710055286
H	-1.0668428812	2.2474186442	1.4897578687
C	-1.7615317758	2.8331256374	-2.2773223348
H	-3.0949032456	1.1657794606	-2.183267549
C	-0.8403165219	3.6658235898	-1.5704894385
H	0.1304644533	4.0615269806	0.2855292031
H	-2.0189510841	3.0729981174	-3.3061833944
H	-0.4303978398	4.5460232744	-2.0592239339
Si	-0.8020221164	-2.0379237763	-0.5992914216
C	-2.4226028124	-2.3508091405	-1.5090571785
C	0.5146620096	-3.285642162	-1.1372098838
C	-1.0038832581	-2.2221837926	1.2744682963
H	-3.2042484765	-1.6627889755	-1.1723884286
H	-2.2964145934	-2.2256493868	-2.5909569923
H	-2.7697496154	-3.3767209877	-1.330379165
H	0.708968395	-3.2420767187	-2.2152507592
H	0.191199534	-4.307538853	-0.9003253654
H	1.4618921252	-3.1066643919	-0.6177403526
H	-1.3583156042	-3.2425065025	1.4801054226
H	-0.0435963503	-2.1031215506	1.7874301613
H	-1.724669647	-1.5248924535	1.7097137758
H	-0.20843858	-0.7295381703	-1.1989223527
S	1.8431339735	0.7181837843	0.3051976241
C	2.8815613107	-0.7174328938	0.6225009361
C	2.1489398709	1.6961425875	1.8219536786
C	2.860661915	-1.4156239674	1.8369652105
C	3.7117919301	-1.1563414742	-0.4159866843
H	1.7079271195	1.2325101469	2.7073479874
H	3.2250718501	1.8248334088	1.9586312242
H	1.6803723181	2.6679787045	1.6576355239
C	3.6738720875	-2.5365770547	2.0105834072
H	2.2121386687	-1.0901708175	2.6448103949
C	4.5113358566	-2.2874554775	-0.2416213914
H	3.7318170199	-0.6077905514	-1.3531279782
C	4.497764297	-2.9776814483	0.9720937814
H	3.6559732453	-3.0706735965	2.956839155

H	5.152682563	-2.6219300143	-1.0525024737
H	5.1257359439	-3.8534447842	1.10929054

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TS_{T1} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.4505069493	0.5389192026	-0.2182267554
S	2.2110879797	-0.0335328016	-1.2937359558
C	1.4934865269	0.9773996115	-0.0140040472
C	3.946986266	0.605609553	-1.6831930858
C	0.6674112659	2.1138794764	-0.4206098797
C	2.1587068824	1.0506854742	1.2745626866
H	4.5767344461	0.5656662953	-0.7922464095
H	4.3596023375	-0.0266268133	-2.4743579217
H	3.8569787196	1.6360688577	-2.0378599853
C	0.5816866949	3.2464403951	0.4785034991
H	0.5813753817	2.3442361098	-1.48413653
C	1.9856881455	2.1203936982	2.103224394
H	2.8239918692	0.2437796227	1.5729634348
C	1.1851755091	3.2451452739	1.6996605154
H	0.0179848028	4.1148667763	0.1453106042
H	2.4895097402	2.1402695931	3.066555969
H	1.0956964951	4.1014368488	2.3626662442
Si	1.6328244946	-1.9613047302	0.0545736186
H	-1.6308058828	1.4819360077	-0.3719804304
C	3.435058416	-2.5334339057	0.2949368406
C	0.853616168	-2.1331248221	1.7815811367
C	0.8526736552	-3.1266301906	-1.213389078
H	3.4386676664	-3.5350852491	0.7459446494
H	3.9788829172	-2.5909846251	-0.6553843311
H	4.0033864105	-1.8750864075	0.9633997316
H	1.0335346071	-1.2524537894	2.4052696069
H	1.2961669108	-3.0025025879	2.2887886282
H	-0.2249225217	-2.2907445075	1.7033504912
H	1.044055285	-4.1643173584	-0.906545551
H	-0.2287415323	-2.9969440922	-1.2971487715
H	1.2969700866	-2.985701765	-2.2044935372
S	-1.8489165374	-1.1653944355	-0.1378179308
C	-2.7455651683	-1.2518463889	-1.7033430382
C	-3.1948432748	-0.6088738082	0.9762270293
C	-3.3975700664	-2.4451590648	-2.0348480767
C	-2.7692322177	-0.1636239913	-2.5807212496
H	-3.5475626516	0.3745514047	0.6602787111
H	-3.9999479332	-1.3477505355	0.967908497
H	-2.7686118621	-0.5392107303	1.9805459262
C	-4.088648438	-2.5422566859	-3.2438897256
H	-3.3600163497	-3.2896917991	-1.3521746873
C	-3.4585192541	-0.2707833132	-3.7894512815
H	-2.2539590087	0.7462365222	-2.2884078006
C	-4.1186856678	-1.4560506403	-4.1218280863
H	-4.5972998322	-3.4673372513	-3.5015717123
H	-3.4784178983	0.5741378146	-4.4727300694
H	-4.6528284837	-1.5355762277	-5.0649599262

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$T1_2$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	1.180098349	1.7091750066	-0.3062873832
C	-0.3424963314	2.4016008342	-0.9727908214

C	-0.6870399682	2.8443224583	0.3081484109
C	-1.227145807	2.6225162792	-2.0270499435
C	-1.8920141737	3.4985626221	0.5696049498
H	0.0161302702	2.6776135365	1.1508648417
C	-2.439922467	3.2781419347	-1.7811322084
H	-0.9833433993	2.2912946107	-3.0333762057
C	-2.7735971985	3.7140451774	-0.4942262184
H	-2.1433600907	3.8373334063	1.5722467727
H	-3.1339380011	3.4505448851	-2.6012617768
H	-3.7186655396	4.2220835993	-0.3203913723
H	1.7107154998	1.2957721042	-1.5818894173
S	2.9092907603	1.0066754934	0.9102231976
C	3.2493475623	-0.7195368639	0.5226952887
C	2.4182996256	0.8600965701	2.6735372168
C	4.3564164713	-1.3498911155	1.1023120671
C	2.4401486149	-1.4039840358	-0.388278863
H	1.5383605455	0.2227557418	2.7864881457
H	3.2506211684	0.4536442001	3.2515401007
H	2.1952247067	1.8691333824	3.0310517499
C	4.6309068845	-2.6819566334	0.7924222973
H	5.0012775985	-0.80348691	1.7850176308
C	2.7306400076	-2.7324702479	-0.7030998831
H	1.6128314971	-0.8771678264	-0.8507283119
C	3.8187516896	-3.3745359153	-0.1097648104
H	5.4867332417	-3.1743398619	1.2459075631
H	2.1026497989	-3.2635863364	-1.4128877572
H	4.0401366845	-4.409636096	-0.35463926

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T2$_1$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.1367278037	0.0375168509	0.5347741965
S	2.4674765721	0.8626135898	-1.2561346941
C	1.5893106654	1.2470480569	0.2987830491
C	3.3854276742	2.4227437773	-1.5782956179
C	0.3945928941	2.2039921044	0.1341309845
C	2.4779187938	1.5182426874	1.435855939
H	4.052244808	2.6600110761	-0.7449851686
H	3.9820444177	2.2604103328	-2.4808983354
H	2.7048435044	3.262709952	-1.7497795507
C	0.2917246227	3.3210572748	1.1302163743
H	0.3169237669	2.5809477431	-0.8939762573
C	2.2673016086	2.5189859041	2.3245636262
H	3.3382722426	0.8648528213	1.5444942347
C	1.1599300418	3.4433137648	2.1524231959
H	-0.4987329442	4.0539422405	0.9797970054
H	2.9405108592	2.6553715232	3.1666208838
H	1.0596722994	4.2719471241	2.8502708644
Si	1.2177068757	-1.8852411776	1.0111136097
H	-0.5864645734	1.5990728758	0.201448973
C	3.1083670804	-1.9139894228	1.2578389031
C	0.5048685302	-2.60838388	2.6386709551
C	0.8501474298	-3.1659381654	-0.3660071398
H	3.4469279616	-2.9516760201	1.3843993326
H	3.6431925023	-1.485126444	0.4039871917
H	3.4069662299	-1.3633300355	2.1578792016
H	0.7101542798	-1.9530856124	3.4945728449
H	0.9671938349	-3.5818454253	2.854191588
H	-0.5795752868	-2.7613448004	2.5858806885

H	1.2836873273	-4.1426560591	-0.1097580831
H	-0.2259382846	-3.3138331956	-0.5213437369
H	1.2832748599	-2.8515420239	-1.3232551876
S	-1.9202933199	-0.8561173217	0.6172998917
C	-2.5854261662	-0.8557676406	-1.0578124577
C	-3.0286173905	0.3619806833	1.4331435773
C	-3.7852566286	-1.5302195298	-1.3138794905
C	-1.8899250054	-0.2317317533	-2.0985256392
H	-2.9794592918	1.3340186709	0.9370679828
H	-4.0530906381	-0.016707361	1.4250800969
H	-2.6847570745	0.4573083325	2.4663416662
C	-4.3012249479	-1.5536309319	-2.6096360712
H	-4.3054296374	-2.0386737244	-0.5069456418
C	-2.4057707024	-0.2721119376	-3.3949636282
H	-0.9478517692	0.2673939523	-1.8951285287
C	-3.6121554031	-0.9258691858	-3.6507830218
H	-5.2344345364	-2.0734161743	-2.8079160909
H	-1.8607921121	0.2076229582	-4.2029384408
H	-4.0118577735	-0.9542424739	-4.6605910746

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TS_{T2} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.4505069493	0.5389192026	-0.2182267554
S	2.2110879797	-0.0335328016	-1.2937359558
C	1.4934865269	0.9773996115	-0.0140040472
C	3.946986266	0.605609553	-1.6831930858
C	0.6674112659	2.1138794764	-0.4206098797
C	2.1587068824	1.0506854742	1.2745626866
H	4.5767344461	0.5656662953	-0.7922464095
H	4.3596023375	-0.0266268133	-2.4743579217
H	3.8569787196	1.6360688577	-2.0378599853
C	0.5816866949	3.2464403951	0.4785034991
H	0.5813753817	2.3442361098	-1.48413653
C	1.9856881455	2.1203936982	2.103224394
H	2.8239918692	0.2437796227	1.5729634348
C	1.1851755091	3.2451452739	1.6996605154
H	0.0179848028	4.1148667763	0.1453106042
H	2.4895097402	2.1402695931	3.066555969
H	1.0956964951	4.1014368488	2.3626662442
Si	1.6328244946	-1.9613047302	0.0545736186
H	-1.6308058828	1.4819360077	-0.3719804304
C	3.435058416	-2.5334339057	0.2949368406
C	0.853616168	-2.1331248221	1.7815811367
C	0.8526736552	-3.1266301906	-1.213389078
H	3.4386676664	-3.5350852491	0.7459446494
H	3.9788829172	-2.5909846251	-0.6553843311
H	4.0033864105	-1.8750864075	0.9633997316
H	1.0335346071	-1.2524537894	2.4052696069
H	1.2961669108	-3.0025025879	2.2887886282
H	-0.2249225217	-2.2907445075	1.7033504912
H	1.044055285	-4.1643173584	-0.906545551
H	-0.2287415323	-2.9969440922	-1.2971487715
H	1.2969700866	-2.985701765	-2.2044935372
S	-1.8489165374	-1.1653944355	-0.1378179308
C	-2.7455651683	-1.2518463889	-1.7033430382
C	-3.1948432748	-0.6088738082	0.9762270293
C	-3.3975700664	-2.4451590648	-2.0348480767
C	-2.7692322177	-0.1636239913	-2.5807212496

H	-3.5475626516	0.3745514047	0.6602787111
H	-3.9999479332	-1.3477505355	0.967908497
H	-2.7686118621	-0.5392107303	1.9805459262
C	-4.088648438	-2.5422566859	-3.2438897256
H	-3.3600163497	-3.2896917991	-1.3521746873
C	-3.4585192541	-0.2707833132	-3.7894512815
H	-2.2539590087	0.7462365222	-2.2884078006
C	-4.1186856678	-1.4560506403	-4.1218280863
H	-4.5972998322	-3.4673372513	-3.5015717123
H	-3.4784178983	0.5741378146	-4.4727300694
H	-4.6528284837	-1.5355762277	-5.0649599262

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T2$_2$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.1618252048	1.1628025767	-0.1973545399
C	0.1075203618	1.9144809867	1.4752636403
C	0.7198228263	2.8400219335	0.6471950072
C	0.1141966876	2.1392186596	2.8496840231
C	1.3542365123	3.9912819776	1.1079833064
H	0.7154348786	2.6617184197	-0.4800090515
C	0.7418050198	3.2895448491	3.350411293
H	-0.353981301	1.4447342007	3.5458855901
C	1.3554298027	4.207055699	2.4912315734
H	1.8282284478	4.6978693414	0.4314916807
H	0.7537143806	3.4728362709	4.4228746386
H	1.8371285977	5.0923154656	2.8978883214
H	-0.0911782892	0.9862975828	-1.7042415185
S	-1.1275674579	-0.6955790635	0.0636477849
C	-2.4413810319	-0.9693477872	-1.1446243292
C	-2.1298371588	-0.6964891583	1.599357609
C	-3.0568720501	-2.225939569	-1.1861106834
C	-2.8216831681	0.0342806369	-2.0374621935
H	-2.841083013	0.1312619415	1.5991251111
H	-2.6545656732	-1.6506741846	1.6858996616
H	-1.4292036694	-0.5806982174	2.4279893801
C	-4.0753769951	-2.4653498918	-2.1089304384
H	-2.7383495918	-3.014162829	-0.5093630694
C	-3.8363046857	-0.2160438066	-2.9629714199
H	-2.2963894574	0.9822009402	-2.0132538965
C	-4.4674352496	-1.4606521107	-2.9971007012
H	-4.5534074153	-3.4405312633	-2.1410761358
H	-4.1306933504	0.5650217956	-3.6584462625
H	-5.2568267525	-1.6516133965	-3.7187913813

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T3$_1$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0592472651	0.2437978583	0.2787091916
S	-1.9184876986	0.2150752127	-0.8060434294
C	-3.1915552938	-0.8476180346	-0.0809291438
C	-2.9236674048	1.7525721544	-0.8758046388
C	-4.2337981564	-1.2833583438	-0.9068221087
C	-3.155196751	-1.2285813077	1.2619316589
H	-3.230457996	2.0560219295	0.1268136191
H	-2.3059877863	2.5291036839	-1.3252850908
H	-3.8026069256	1.5690129711	-1.4979078809
C	-5.246675876	-2.0882389345	-0.3822371072
H	-4.2480774752	-1.0033854895	-1.9566946341

C	-4.170633536	-2.0333125302	1.7810437882
H	-2.3177859194	-0.9167754024	1.875782506
C	-5.2179406518	-2.462231534	0.9627519954
H	-6.0511509946	-2.4299584458	-1.0279021462
H	-4.1402718628	-2.3272088023	2.8268359197
H	-6.0048496099	-3.0914935214	1.3695769265
Si	0.5636718899	2.4447222824	-0.2678577986
H	-0.4250462373	-1.2042902176	0.5891753473
C	0.4209375189	2.8573525398	-2.1432140883
C	-0.3945371012	3.7936667058	0.7138212888
C	2.3953065888	2.90807835	0.0873812572
H	0.6641112776	3.9121592215	-2.3330181808
H	1.1472837025	2.2505049603	-2.6997499684
H	-0.5609517732	2.6597773213	-2.5898631865
H	-1.4829234482	3.7505964572	0.5961614054
H	-0.0688351551	4.7980240291	0.4088109856
H	-0.1817443716	3.6949061216	1.7863944482
H	2.5799217149	3.9490208565	-0.2121510417
H	2.6474659459	2.8210518867	1.151025054
H	3.0983343157	2.2790680197	-0.4726248307
S	1.82395322	-0.0996609969	1.3288202263
C	2.963081783	-0.7747578637	0.1033323906
C	1.6583735173	-1.5662506132	2.4183723089
C	4.3181435853	-0.4404935379	0.1865600681
C	2.5006113725	-1.6232068756	-0.9095748074
H	1.2871988077	-2.4189910192	1.8483630669
H	2.6268844021	-1.7809489284	2.8787266778
H	0.9317953814	-1.3035429901	3.1912515804
C	5.2162123625	-0.9654508255	-0.7454103177
H	4.6620248371	0.2296426143	0.9685064401
C	3.4055052846	-2.1447640324	-1.8344285222
H	1.4432600358	-1.8656873711	-0.9595306918
C	4.7615040052	-1.8169740813	-1.753972691
H	6.2692424799	-0.7050894971	-0.683649063
H	3.0490525479	-2.8027556995	-2.6222016818
H	5.4620817132	-2.2219552806	-2.4791401013

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TS_{T3} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.1852564739	0.1442632993	0.1524911942
S	-2.0038980179	0.3191848304	-1.0772379566
C	-2.2790771863	-1.0809374285	0.2671081313
C	-3.1540880305	1.6595764924	-0.6055843503
C	-2.9032294938	-2.2846532892	-0.2014984038
C	-2.6233093812	-0.6542218753	1.5861228475
H	-3.6653653562	1.3602888248	0.314721395
H	-2.6104278701	2.5902656583	-0.4401733974
H	-3.8839151241	1.7850809436	-1.4085308676
C	-3.6681153626	-3.0625502274	0.6454083794
H	-2.7323444984	-2.5995537234	-1.2268377594
C	-3.4005531795	-1.4671574121	2.4170617925
H	-2.2620349875	0.2987953622	1.9627634363
C	-3.9207587203	-2.6805976126	1.9761786085
H	-4.099422675	-3.9829717173	0.2568228068
H	-3.6124654462	-1.118957153	3.4262720722
H	-4.5337495849	-3.2969984612	2.6258664113
Si	0.5389334003	2.3322299199	0.2121199286
H	-0.8299201116	-1.3083964648	0.0517687959

C	0.2877051949	3.2013515592	-1.47533225
C	-0.3401790553	3.3842734457	1.5539943282
C	2.4082877456	2.5387302932	0.5790859779
H	0.5876085598	4.2568462963	-1.4202641182
H	0.9073900796	2.7229919804	-2.2442925748
H	-0.7485912991	3.1712241064	-1.8327093654
H	-1.4317359331	3.3958086942	1.4483653908
H	0.0054583917	4.4268476071	1.5189398406
H	-0.1149118929	2.9970643987	2.5558117376
H	2.6892922165	3.6005382042	0.5544495887
H	2.6732104093	2.1505763118	1.5701399674
H	3.0303884345	2.0175093531	-0.1590846336
S	1.4043639123	-0.6370095516	1.4255098152
C	2.7393233352	-1.2815380156	0.3981146589
C	0.7615252231	-2.1941792793	2.1553064421
C	4.0556958528	-1.1143639757	0.8386368865
C	2.4735303133	-1.9256980632	-0.8156330279
H	0.5512514577	-2.9219299404	1.3700975871
H	1.4928152123	-2.5838698142	2.867350406
H	-0.1702983872	-1.9425385467	2.6677132642
C	5.1097084921	-1.6047326712	0.0646046627
H	4.2504415928	-0.6012540165	1.7754239961
C	3.531602263	-2.4167212167	-1.58036079
H	1.4462163198	-2.0363750971	-1.1513835131
C	4.8488903482	-2.256372452	-1.1419837803
H	6.1331093078	-1.4744336003	0.4050781645
H	3.3270116783	-2.9174043901	-2.5226118443
H	5.6708045169	-2.6348900659	-1.743312661

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T3$_2$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0995579579	0.6074821562	-0.5360717654
S	-1.4993015315	1.1643579624	-1.9913236082
C	-3.1063688867	1.5522363653	-1.1729253121
H	-3.4459489123	0.7421903594	-0.5228312718
H	-3.0325618725	2.473175002	-0.5886386019
H	-3.8487909873	1.7008591623	-1.9620299082
Si	0.661811456	2.6210775634	-0.0406231674
C	1.707195658	3.2933348669	-1.4820707924
C	-0.6894071298	3.8899472212	0.3846703385
C	1.8095565447	2.5723575538	1.4890918801
H	2.1283284582	4.273648925	-1.2187731442
H	2.545509115	2.6264611089	-1.7165860682
H	1.1030431047	3.4102717131	-2.3877327845
H	-1.3100408745	4.1203172289	-0.4873533328
H	-0.2268735716	4.8247126266	0.730398975
H	-1.3466050646	3.5342417481	1.1873533723
H	2.1763818246	3.5868402592	1.6998218042
H	1.2890267348	2.2156166984	2.3855503492
H	2.6862740111	1.9319977151	1.3354675555
S	1.1655704414	-0.6522348329	0.7249094432
C	2.7589426089	-0.9014240064	-0.0821942303
C	0.4110445784	-2.3093058254	0.4570954214
C	3.8616616528	-1.2707371685	0.6950726181
C	2.8962556401	-0.7133829912	-1.4627200246
H	0.3024741196	-2.5193398502	-0.6093385507
H	1.0334189213	-3.0699223065	0.9340165001
H	-0.5746837086	-2.2931541283	0.9291507563

C	5.1020794827	-1.4656778201	0.0841772828
H	3.7487124972	-1.3995365902	1.7675392759
C	4.1386278858	-0.9110144157	-2.0657216719
H	2.0342634597	-0.4077854258	-2.0482857358
C	5.2406285261	-1.2876898375	-1.2938971382
H	5.9596930852	-1.7518422898	0.6865913504
H	4.2453767784	-0.7649341736	-3.1368355398
H	6.2078129124	-1.437177574	-1.7655992746

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T4$_1$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.5842123524	0.4601044068	0.0596093953
S	-0.8690674339	-1.205573002	-0.1589091016
C	-2.563019794	-0.7786410603	-0.5720683004
C	-0.4697888582	-2.4849469311	-1.3967416344
C	-3.3234158346	-0.1822230313	0.4436345049
C	-3.1386016187	-0.9980495642	-1.8290405972
H	-1.2533861551	-3.2468997086	-1.3998868723
H	-0.3452813862	-2.0653167002	-2.3981516817
H	0.4714893265	-2.9292738469	-1.0664291231
C	-4.6420214443	0.1970627844	0.1990920721
H	-2.881306859	-0.0213640485	1.4229415568
C	-4.4655344799	-0.62645327	-2.0611971545
H	-2.5646041621	-1.4504363214	-2.6306967115
C	-5.2203013287	-0.0261792234	-1.0530856725
H	-5.2222604054	0.658187703	0.9938012216
H	-4.9044917436	-0.8032043223	-3.0396281219
H	-6.2504773793	0.2632436078	-1.2398953741
Si	-0.0448792982	2.4993284874	-0.9046204387
H	-0.4743744441	1.5630375481	0.3498434655
C	0.6676239589	4.0708447215	-0.1216248611
C	0.9472697284	2.0852774737	-2.485501822
C	-1.8047725021	2.8450868772	-1.5229923846
H	0.6346715411	4.9054938189	-0.8335260446
H	0.0916421432	4.3658267502	0.7633357496
H	1.7099926802	3.9394923271	0.1886998007
H	2.0168296231	1.9421104313	-2.3034693983
H	0.8361792735	2.9182729331	-3.1949280505
H	0.5663822077	1.1856579638	-2.9820421168
H	-1.8052376536	3.6423300271	-2.2775685286
H	-2.2341669958	1.9484917789	-1.9851082092
H	-2.4777402875	3.1488107376	-0.7129938901
C	2.4076156818	0.9757971232	0.5816983152
C	2.3724720088	-0.4087697616	0.1513831786
C	2.4938535749	1.2479727457	1.9940905167
H	2.7972295943	1.7363071939	-0.0947258233
C	2.5609511487	-1.4455493669	1.147002946
H	2.7017409863	-0.6480019829	-0.8613080341
C	2.5361552766	0.2262787671	2.9064353689
H	2.5366857291	2.281671828	2.3288810787
C	2.59130892	-1.1381386203	2.4867650173
S	2.7911779131	-3.0872678422	0.4839693314
H	2.5812856002	0.4456064407	3.9704573455
H	2.7020440982	-1.9103732541	3.2400084889
C	2.9622364539	-4.1340011021	1.9644834148
H	2.0610965648	-4.1003870356	2.5829765442
H	3.1075429194	-5.1537976908	1.5989699784
H	3.8327827594	-3.8403657897	2.5575416559

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TS_{T4} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0652889113	0.2306721388	0.6694200387
S	-1.1560776778	-1.4168985349	1.86491858
C	-2.3724379486	-0.3038348905	0.6103148883
C	-1.2087767842	-3.0265990879	1.0096021397
C	-3.3232983224	0.456714016	1.3687689252
C	-2.8723962963	-0.9756052519	-0.5474830242
H	-2.1912303507	-3.151907372	0.5413582108
H	-0.4215432951	-3.1305270471	0.2588671792
H	-1.0780341991	-3.7925485449	1.7786506919
C	-4.6450154407	0.5501380528	0.9727477149
H	-2.9903373436	0.9621818531	2.2709236495
C	-4.211342881	-0.8678798071	-0.9180833122
H	-2.1849358207	-1.525529096	-1.1825205607
C	-5.1166383622	-0.1144944356	-0.1709159633
H	-5.3304176484	1.138891422	1.5783853007
H	-4.5428489225	-1.3808803267	-1.8183375188
H	-6.1573497238	-0.0370554835	-0.4689722047
Si	-0.0281771182	2.0140951134	-0.7577552363
H	-1.4495155439	0.5652951578	0.1611671608
C	-0.7673046348	3.5653431913	0.0781838705
C	1.7415046824	2.5014672017	-1.3167104264
C	-0.9600564074	1.6981446959	-2.3940848193
H	-0.749563021	4.4281069121	-0.6012281491
H	-1.8084844175	3.4014835204	0.3815709178
H	-0.2022999745	3.8418801394	0.9775804998
H	2.4279253009	2.7190744604	-0.4892656333
H	1.6878098129	3.4075431276	-1.9354877366
H	2.2016774861	1.7199702103	-1.9345636362
H	-0.9546708899	2.5954290653	-3.0274481087
H	-0.4781527308	0.89245649	-2.9630660754
H	-2.0042826253	1.4065558998	-2.2328471609
C	1.7456731069	0.7157917294	1.7562816202
C	2.0353927528	-0.2629888718	0.7753162986
C	1.6727910435	0.3443359913	3.1199128801
H	1.8312248888	1.767159066	1.5043566117
C	2.2867035847	-1.606839871	1.1735910517
H	2.3446153696	0.0475722763	-0.2179550716
C	1.8634113949	-0.9775610629	3.479394228
H	1.4775820179	1.100012767	3.8746006297
C	2.1704243999	-1.9577246437	2.5142227157
S	2.7260552581	-2.7289740577	-0.135172164
H	1.7958452534	-1.2731434737	4.5229053063
H	2.336004567	-2.9787521985	2.8394091525
C	3.1776033163	-4.2580874504	0.7475499951
H	2.3178957358	-4.7028138296	1.2562665016
H	3.5285841791	-4.9506591894	-0.0215582866
H	3.9865453208	-4.079636881	1.4612611893

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$T4_2$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	1.0303513461	0.4522834964	0.6007107511
S	-1.0438563648	-0.0811832608	0.8167164409
C	-1.1629118019	-1.6904875347	-0.0752397194
H	-0.9925613216	-1.5657859875	-1.1482775592
H	-0.4553201608	-2.4275227225	0.3155760431

H	-2.1778482613	-2.0717011572	0.0702233401
Si	0.3648567151	1.8208165028	-1.0174867449
C	-0.7033229509	3.237442547	-0.3365701111
C	1.909773527	2.6717901724	-1.7723298162
C	-0.4863238662	1.0000540182	-2.5045237791
H	-0.9167725521	3.9622726481	-1.1342673707
H	-1.6530080712	2.865231923	0.0582827178
H	-0.1885336028	3.7775499655	0.4675358126
H	2.5376060294	3.1843744955	-1.0338732097
H	1.564908977	3.4343936514	-2.4846594624
H	2.5437507052	1.9741128332	-2.3325802119
H	-0.5858064386	1.7265556379	-3.3225538407
H	0.0980892952	0.1553252373	-2.889619539
H	-1.4847642577	0.6359491137	-2.2449962462
C	2.8108699452	1.1814473086	1.3108004778
C	3.0314364453	0.2395782526	0.2700210897
C	2.5460828707	0.728958485	2.6313410543
H	2.9864283295	2.2361461751	1.125679154
C	3.0177290078	-1.1631065189	0.5620103417
H	3.3983347073	0.5752606716	-0.693845056
C	2.4470074899	-0.6304648219	2.8731022383
H	2.3954999427	1.4470583114	3.4305347686
C	2.6777202697	-1.5789640941	1.8462979464
S	3.448926838	-2.2397584873	-0.7814400694
H	2.1891967007	-0.9888970525	3.8650142936
H	2.6079684508	-2.6328909207	2.0886147392
C	3.2646501343	-3.9047442153	-0.0655308391
H	2.2334549533	-4.0947898354	0.2448640815
H	3.5261300698	-4.5997673881	-0.8672871196
H	3.9479378996	-4.0590184497	0.7740424041

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$TS_{5A\text{-}6A}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.6449949475	-0.1462385033	-0.0982196221
S	0.6908384138	-2.2717515171	-0.3603876395
C	2.4844542658	-0.0095975643	0.1292320658
C	2.2739758382	-2.9513723667	-0.9909121339
C	3.0771100118	-0.2214634572	1.3811639189
C	3.2868786241	0.3991997424	-0.9434827356
H	2.5755684058	-2.4728375347	-1.9256348673
H	3.0690688695	-2.828717414	-0.252354337
H	2.1130909947	-4.0175783784	-1.1724076907
C	4.4503672492	-0.0215926429	1.5551664867
H	2.476425294	-0.5571235889	2.2221784526
C	4.6613062605	0.5953607421	-0.7652613634
H	2.8555306348	0.5536858762	-1.9297382145
C	5.2471638368	0.389225009	0.4840968842
H	4.8961936751	-0.1928153746	2.5324151841
H	5.2709897748	0.9104094134	-1.6091682856
H	6.3144320691	0.541233745	0.6213375789
Si	-2.9932773057	-1.8790187124	0.1363580521
H	-1.8942096849	-0.8465265033	0.1909472422
C	-4.6250466057	-0.9917740073	0.5173426696
C	-3.0224226256	-2.6062836288	-1.6049643557
C	-2.6247318387	-3.1878231762	1.4450276502
H	-5.4628627276	-1.7002509665	0.49874869
H	-4.6106144765	-0.5258606442	1.5097592043
H	-4.8435569984	-0.2070975992	-0.2169331095

H	-3.2681810978	-1.8442663142	-2.3544660886
H	-3.7688364033	-3.4061931482	-1.6871761274
H	-2.0409907978	-3.0228092435	-1.8550759969
H	-3.36517823	-3.9969281306	1.4147636078
H	-1.6329849787	-3.6211325454	1.2776639033
H	-2.6408994156	-2.7601898737	2.4547561232
C	0.1982175835	1.673485273	0.7486133402
C	0.1706329979	1.7412627366	-0.6407033541
C	-0.9632482135	1.6386642955	1.7359715065
H	1.1380154349	1.975356202	1.2061493272
C	-1.0472787099	1.7701291439	-1.5425216344
H	1.0743844558	2.1261452067	-1.1141335456
C	-2.3276264653	2.1847683846	1.2504306577
H	-0.6460273264	2.2329743728	2.6027719923
H	-1.1153877503	0.621481666	2.1243819176
C	-1.5842227301	3.205607242	-1.7519236602
H	-1.8378847971	1.1157749106	-1.1713022249
H	-0.7664584771	1.3733446475	-2.5265024777
C	-2.2754303536	3.5961383631	0.7108585004
H	-2.7662651661	1.4997700774	0.5224049998
H	-3.0048962104	2.1658829836	2.11366705
C	-1.972383564	4.0032620222	-0.5282203743
H	-0.816671032	3.7801827915	-2.2902926329
H	-2.4406966778	3.1587520838	-2.44323105
H	-2.5037598283	4.3761176798	1.4376970845
H	-2.0056501492	5.0787002247	-0.7083045684

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6A B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.4049659981	-0.3400218886	0.1628119516
S	0.6871244344	-2.4874967766	0.2173924775
C	2.2530687741	-0.0660957451	0.02985316
C	2.3985111093	-3.1193880968	0.0404726791
C	3.0442803646	0.0924294318	1.1763652314
C	2.85941229	0.0730339684	-1.2268927207
H	2.8383846831	-2.8209663761	-0.9134964541
H	3.0390553808	-2.7686589066	0.8523347084
H	2.3317764792	-4.2103800213	0.0799117562
C	4.4079473453	0.38669665	1.0682445852
H	2.6062981613	-0.0284012934	2.1644958835
C	4.2231618691	0.3671739639	-1.3336850822
H	2.2753760651	-0.059155276	-2.13504678
C	5.0026915622	0.5274026017	-0.1867927618
H	5.004309783	0.5034278943	1.9705487
H	4.6741567668	0.4694358513	-2.3183810368
H	6.0621466358	0.7549706343	-0.2701809958
Si	-2.7042701316	-1.7206062711	-0.1231409395
H	-1.5437617437	-0.7985538742	0.2625059391
C	-4.2944784856	-0.7012507198	0.0122415378
C	-2.4293070418	-2.283424654	-1.8980899908
C	-2.7403675995	-3.130183233	1.1218690297
H	-5.1550433202	-1.3446288514	-0.2134742036
H	-4.4418216849	-0.3030913485	1.0224908433
H	-4.3234842102	0.1376106076	-0.692156421
H	-2.3991296868	-1.4309763468	-2.586915349
H	-3.2428408707	-2.9446914352	-2.222258247
H	-1.4838191447	-2.8280794865	-1.9809714189
H	-3.5112378506	-3.8622849531	0.849644486

H	-1.7722649509	-3.6383756657	1.1548665699
H	-2.9700215131	-2.762708316	2.1289800334
C	-0.002106678	1.5256967457	0.9292021523
C	-0.0800679663	1.558898285	-0.4588883963
C	-1.1283230502	1.6071149078	1.9533106977
H	0.969015983	1.7922474211	1.340636415
C	-1.3199933157	1.7181330659	-1.3110596787
H	0.8289151941	1.872217463	-0.9714485516
C	-2.420850149	2.3436594783	1.5188346549
H	-0.7151710371	2.1268864105	2.8270001844
H	-1.4044043469	0.6074813352	2.3168498089
C	-1.6692073257	3.2099429766	-1.5285959938
H	-2.1740787552	1.1869841192	-0.892561348
H	-1.1370030686	1.272329932	-2.2978193297
C	-2.1921582125	3.7274375088	0.9539827166
H	-2.9835194455	1.7267469938	0.8161134073
H	-3.0575710316	2.4283929114	2.4087610043
C	-1.8889095963	4.070663628	-0.3045592546
H	-0.8578204687	3.6686091419	-2.1117222987
H	-2.5558181156	3.2701067592	-2.180078961
H	-2.2763645425	4.5410700427	1.6748209713
H	-1.7778135396	5.1375188065	-0.5034313708

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TS_{6A-7} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.2848330984	-0.050300093	-0.1189142452
S	-1.5088519492	1.5520497735	-1.0071481969
C	-1.7629743629	-1.2271944733	0.0983622624
C	-2.2695601686	-1.5140425799	1.3776263372
C	-2.4067176718	-1.8244985309	-0.998692655
C	-3.3738403404	-2.3560776018	1.555658402
H	-1.8081143181	-1.0756181624	2.2621907403
C	-3.5036427817	-2.6753465026	-0.8279805402
H	-2.0589888104	-1.616166651	-2.0092836039
C	-3.9935351726	-2.9438556999	0.4523468322
H	-3.7462269372	-2.5531844902	2.5589303511
H	-3.978791115	-3.1250267735	-1.6975022456
H	-4.8481305882	-3.6020023462	0.5873538135
C	-3.1846234942	1.7017565957	-0.2793078482
H	-3.135792212	1.9232635842	0.7886020435
H	-3.7069273545	2.511476212	-0.7944577135
H	-3.713817689	0.758986139	-0.4279019448
H	0.8174534899	1.1674631119	-0.2672580478
Si	0.3150092185	2.8081663397	0.0572722594
C	1.1517048877	3.5333940008	-1.4786845381
H	1.3848154365	4.5900431979	-1.2941713569
H	2.0889543875	3.0146079766	-1.7065831024
C	-0.9517190411	4.0674631783	0.7534103541
H	-1.6553263472	4.4132361321	-0.0114927628
H	-0.4219212997	4.9410409863	1.1569413699
C	1.5498547759	2.8045375764	1.5226119122
H	1.7896972667	3.8423444697	1.7904834073
H	1.1158966373	2.3416473463	2.4182284636
H	0.5070235499	3.4811112419	-2.3612435482
H	-1.5382095883	3.6435435576	1.5785663436
H	2.4840625039	2.2845878168	1.2886267573
C	1.048586683	-1.3396234907	0.8679594286
C	1.0433266648	-1.5658981257	-0.5001808693

C	2.126099142	-0.7374559705	1.7501487326
H	0.3453987249	-1.9534796663	1.4281744255
C	2.0752369328	-1.1660773356	-1.5342394464
H	0.3756472789	-2.3561861415	-0.8419511677
C	3.5125964786	-0.4756816397	1.123870411
H	2.2601256907	-1.4442999446	2.5816250969
H	1.7630023094	0.1860726485	2.215343693
C	3.2113890688	-2.2028115679	-1.6619881942
H	2.481045788	-0.1739496363	-1.3380390693
H	1.5731882232	-1.0979452354	-2.5077170467
C	4.2239923815	-1.7359647769	0.6771513335
H	3.428484125	0.2531847237	0.3147993514
H	4.1268002108	0.0090796182	1.8928338255
C	4.0899203802	-2.4355646791	-0.4569351783
H	2.7735677521	-3.1701603472	-1.9503786384
H	3.8467279501	-1.9152176004	-2.51465092
H	4.9284563082	-2.1367172142	1.406698097
H	4.7156900937	-3.3245019505	-0.5517421647

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5B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.5322847819	0.7593729549	-0.0190712105
S	-3.6289869646	0.7549073846	-0.1890952164
C	-1.3610372844	-1.0823710942	-0.0206317025
C	-4.4564636787	-0.8806688597	-0.2425241638
C	-1.1848257278	-1.7598119689	1.1998442105
C	-1.0560563258	-1.7718686121	-1.2084251978
H	-4.1390816635	-1.4661373515	-1.1077372944
H	-4.2742779742	-1.4548057043	0.6682184085
H	-5.5280119481	-0.6706739698	-0.3250602087
C	-0.6856940676	-3.0656301809	1.2343019306
H	-1.449492216	-1.2741102777	2.1371657456
C	-0.557488927	-3.0777689877	-1.1762107038
H	-1.2195545355	-1.2953743098	-2.1730122539
C	-0.3678661683	-3.726652548	0.0459343138
H	-0.5517734913	-3.5686430929	2.189532847
H	-0.3230526158	-3.5904823311	-2.1065731614
H	0.0128959353	-4.744541731	0.0713209449
C	2.2824728371	3.5110761661	0.4766099977
C	2.2850659146	3.0758319604	-0.789395689
C	1.4885729731	3.0715261014	1.679200045
H	2.9786483384	4.3192565645	0.7069120005
C	1.4398973498	2.0122570044	-1.4609733424
H	2.9706794272	3.5873088895	-1.4653131036
C	0.3627783154	2.0378962094	1.4776908792
H	1.0579387075	3.9674209213	2.151177786
H	2.1906580175	2.6673659277	2.425325093
C	0.0160181805	2.4925796047	-1.8095514077
H	1.391443208	1.0850138723	-0.8813564135
H	1.9294132948	1.7364660466	-2.4020756731
C	-0.8357451645	2.5480561516	0.6893104571
H	0.7833038155	1.1243485813	1.0409498959
H	0.0005782886	1.742963267	2.4691767073
C	-0.9764523475	2.6821220406	-0.6781574214
H	0.0954327486	3.4614827151	-2.3246712234
H	-0.4256655379	1.810550629	-2.5504235531
H	-1.6061255345	3.0161274525	1.300371753
H	-1.8787593971	3.199673575	-1.0027930753

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$TS_{5B\text{-}6B}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.8330153419	-0.0406958332	-0.0343083318
S	-2.921510166	0.3021954371	0.1450992486
C	-1.0662530039	-1.8951318596	-0.0996981389
C	-4.0305308091	-1.155300571	0.0866440442
C	-1.05554866	-2.691304023	1.060957893
C	-1.0722619447	-2.5577605949	-1.3412794527
H	-3.933090362	-1.7017139507	-0.8535471574
H	-3.8520523645	-1.8371705513	0.9201986183
H	-5.045970779	-0.7519776412	0.1632989806
C	-1.0157492073	-4.08767426	0.986408723
H	-1.0932225687	-2.2209923049	2.0419131466
C	-1.0342547333	-3.9541267242	-1.4224119082
H	-1.1210483314	-1.9844832165	-2.2655645952
C	-1.0033288087	-4.7242942409	-0.2574399987
H	-1.0078571354	-4.678889639	1.8998157273
H	-1.0392336552	-4.440092222	-2.3958590157
H	-0.9850904415	-5.8096001177	-0.3176883486
Si	2.8786857732	-1.8094965647	0.1526445943
H	1.7315109811	-0.8664954998	-0.1004975993
C	4.4931687743	-0.8253384418	0.0196037613
C	2.6896371141	-2.5145076251	1.8951802972
C	2.8281415102	-3.1698948324	-1.154803041
H	5.355185233	-1.4800972252	0.1999119995
H	4.6193609325	-0.3827309846	-0.9753582746
H	4.5407954175	-0.0131745289	0.7549361018
H	2.6980984351	-1.7224428709	2.6536088037
H	3.5101459158	-3.2046339701	2.1281937547
H	1.747316548	-3.0639724948	1.9906297177
H	3.6456800384	-3.8860514066	-1.0036546731
H	1.8814739583	-3.718598407	-1.1129388531
H	2.932548677	-2.7569365489	-2.1653030973
C	2.0483375116	3.9977639628	0.518470084
C	2.3183929071	3.6000846622	-0.7314995348
C	1.6444211362	3.1933906384	1.7336885722
H	2.1240534939	5.0680368635	0.7151919176
C	2.3128517023	2.1936490394	-1.2864756116
H	2.5663423465	4.3813019985	-1.4503519941
C	1.0291344935	1.7925910438	1.5008661332
H	0.9182849896	3.794221328	2.2995847183
H	2.5106663699	3.0866707257	2.4059884172
C	0.9234217822	1.6905576782	-1.7521131594
H	2.7397935298	1.4910958718	-0.5685972768
H	2.9757965657	2.1579047522	-2.1602713488
C	-0.1921474009	1.8615448501	0.6101834844
H	1.7791475055	1.1065716666	1.1061207875
H	0.7343445144	1.3905857214	2.4784769552
C	-0.2315720392	1.8300067337	-0.7679542072
H	0.6337547393	2.2517717522	-2.6492884079
H	1.0292068454	0.6477560939	-2.0870753023
H	-1.0741378653	2.2652536442	1.1060281218
H	-1.1527826037	2.188691057	-1.2225356849

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6B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.0791169201	-0.2907949469	0.0358564229
S	0.3308611661	-2.3480038739	-0.4294992762
C	-1.9360284159	-0.6227893256	0.0062719673
C	-2.6993195809	-0.4578738979	-1.1635474843
C	-2.6332214833	-0.8830779353	1.1997642912
C	-4.0977259807	-0.5201643464	-1.1402043789
H	-2.2009472367	-0.2942113418	-2.1178080147
C	-4.029982557	-0.9521095016	1.229439155
H	-2.0842665367	-1.043552278	2.1260399769
C	-4.7697422276	-0.7649171822	0.0590306782
H	-4.6602869282	-0.3867597197	-2.0620840504
H	-4.5408966467	-1.1552737331	2.1684759569
H	-5.8552120265	-0.8212946234	0.0796017195
C	-1.1034773148	-3.4446968812	-0.7370698364
H	-0.6801689197	-4.4336355958	-0.9415903396
H	-1.7576886582	-3.5086912691	0.134762345
H	-1.6895546033	-3.1222751234	-1.6002260911
H	-0.519562347	1.3594456086	0.5954770506
Si	-1.0875735441	2.7399199321	0.2914966678
C	-2.7439397192	2.8514288809	1.1717572806
H	-2.6307560692	2.7073711028	2.2521375271
H	-3.1986228141	3.8372028269	1.0112281403
C	0.1864023773	3.9409644382	1.0024090727
H	1.1702943567	3.8135257622	0.5359229507
H	-0.1263171291	4.9789915173	0.8323246895
C	-1.2486211329	2.9627903249	-1.5716753577
H	-1.6293673079	3.9680757328	-1.7931248742
H	-0.2877577492	2.8540400071	-2.0872704528
H	-3.4355273174	2.0881263818	0.8016229267
H	-1.9506187276	2.2376499977	-1.9946213654
H	0.3075876026	3.8071338554	2.0836225807
C	1.8598572946	0.5389727624	-0.5038924291
C	1.8736130104	0.2132451097	0.8316279688
C	2.6002590464	-0.0856219515	-1.6738313434
H	1.4962276383	1.5417402552	-0.7341353789
C	2.6287289658	-0.8954649999	1.5319275446
H	1.541168265	0.9976371947	1.5143562164
C	3.7644439025	-1.0466377454	-1.349508482
H	3.000200974	0.752393431	-2.2629439534
H	1.8902670639	-0.6049972471	-2.3283308011
C	4.0747530901	-0.4814814378	1.8770193192
H	2.6151021518	-1.8213604556	0.960483949
H	2.1092583246	-1.1243790101	2.470577091
C	4.8957778073	-0.398259182	-0.579669595
H	3.377567928	-1.9358185616	-0.8487116821
H	4.1606579761	-1.4005614035	-2.309331405
C	5.0103951471	-0.1666556119	0.7347038189
H	4.0446435546	0.3990160656	2.5373454773
H	4.5219706698	-1.2786870222	2.4918913523
H	5.7238690313	-0.051981184	-1.1995027311
H	5.9294095497	0.3243692004	1.0598181855

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TS_{6B-8} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.164256040973	0.068507637015	-0.208161871228
S	0.187384422533	-1.836432408538	-1.281790764450
C	-2.016362069395	-0.447038175629	0.319615433256
C	-3.109840079837	-0.332100724359	-0.557149442353

C	-2.206430840503	-1.155478304923	1.519856920909
C	-4.330102458447	-0.947679944298	-0.272273665017
H	-3.002678367889	0.225124871888	-1.484826479597
C	-3.425790549406	-1.771442577302	1.805991711856
H	-1.393625695816	-1.236457419453	2.237564778385
C	-4.492784665028	-1.673024668171	0.909918578871
H	-5.154234934921	-0.860089441057	-0.976117177910
H	-3.543569266028	-2.326064514423	2.733829738313
H	-5.443761086302	-2.148096803774	1.134979972983
C	-1.225050270560	-3.001344360928	-1.296474924437
H	-0.889244669942	-3.890334056186	-1.838693521289
H	-1.517822781351	-3.296878990399	-0.285777454724
H	-2.096678993807	-2.584464127363	-1.807115142638
H	-1.304613430016	0.766448315375	0.520697435858
Si	-0.813953106572	2.436909989796	-0.085383025731
C	-2.511642639731	2.990892069704	0.562483917540
H	-2.585447438186	2.889389636421	1.651621636505
H	-2.674964250800	4.048106111466	0.315186083468
C	0.454605451794	3.558460476535	0.776635514960
H	1.494652240030	3.391765926781	0.481799398211
H	0.205170968812	4.599473693463	0.531058387904
C	-0.825368051132	2.724623846265	-1.965080851254
H	-1.063501470431	3.779014911939	-2.162535442881
H	0.128946960216	2.495014529420	-2.448285310296
H	-3.329637485193	2.412105943086	0.122303872453
H	-1.597055006885	2.118576301899	-2.452807414377
H	0.389314143303	3.462388274139	1.866843814490
C	1.909377608199	0.674191563812	-0.583878598262
C	1.666146055127	0.399917339500	0.751204308511
C	2.776925143306	-0.067415554942	-1.589901520511
H	1.770712489949	1.716986756970	-0.862776836235
C	2.084510628077	-0.820381857036	1.543344875922
H	1.442288227957	1.258342033707	1.382815956718
C	3.752213418497	-1.134528430194	-1.043132546457
H	3.368280221781	0.709203732774	-2.095832965921
H	2.158831624856	-0.530966180708	-2.366509091720
C	3.478548106215	-0.636215793954	2.183171137065
H	2.037542145719	-1.721320111382	0.935683696300
H	1.364176047455	-0.969952962067	2.358642683628
C	4.769149522016	-0.597798185262	-0.059551480249
H	3.184603575388	-1.972662445486	-0.636285973376
H	4.291623076693	-1.539320611224	-1.908596766428
C	4.649069232246	-0.395872794148	1.259099394631
H	3.432627958385	0.206047340342	2.890250036043
H	3.686671708228	-1.518745342866	2.808608229897
H	5.727799753627	-0.321530234807	-0.500770456196
H	5.526587918740	0.000651718581	1.772580208860

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8 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-1.1415669267	0.6737439191	0.5065893797
S	0.3878075268	1.045296048	1.9592945115
C	1.0808880922	-0.6682254825	2.0595991353
H	0.3179917613	-1.4217154898	2.2756446707
H	1.6044720815	-0.9402103306	1.1383636085
H	1.8059514401	-0.6780860034	2.8782595152
Si	-0.3810824105	2.3591058313	-0.7364659922
C	1.0711218865	1.7582757363	-1.8028957165

H	0.8031535401	0.8874055249	-2.4125051128
H	1.388040509	2.5572298779	-2.4872156631
C	-1.7685465907	2.9633315103	-1.9023932524
H	-2.6085214177	3.3876784387	-1.3396546025
H	-1.3617526599	3.7681858799	-2.5305661806
C	0.1188501969	3.9040517563	0.2444489638
H	0.3273248075	4.7269946695	-0.4533184963
H	-0.6864422013	4.2357872399	0.9104810731
H	1.9271690794	1.4862484768	-1.176889813
H	1.0075242856	3.7258587791	0.855180983
H	-2.1651657342	2.1939591462	-2.5733853633
C	-3.0046362198	0.2689246465	-0.0549637386
C	-2.0785464956	-0.3466684281	-0.9083029428
C	-3.791850783	-0.3032886095	1.1188184674
H	-3.4612820043	1.1759153153	-0.4516022946
C	-1.529473449	-1.761788376	-0.8357002813
H	-1.9674657671	0.0988875298	-1.8959284531
C	-3.7027830387	-1.8204350743	1.3917244368
H	-4.847876043	-0.0558878025	0.9383165619
H	-3.5253472059	0.2368674787	2.0400783869
C	-2.443036272	-2.8211802505	-1.4851904722
H	-1.295113655	-2.056060614	0.1909897578
H	-0.5711808111	-1.776628835	-1.3706668982
C	-4.3169382438	-2.6692825116	0.2985065894
H	-2.6693341823	-2.1091815784	1.6032576159
H	-4.2516773464	-2.0122815512	2.3215852683
C	-3.8004438613	-3.0613153995	-0.872905625
H	-2.5934678151	-2.5479709806	-2.5404696142
H	-1.8969588602	-3.7775792462	-1.5157154439
H	-5.3452406217	-2.9745176678	0.4944121369
H	-4.4501095906	-3.667308573	-1.5065641053

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6C B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.1013788135	-0.1991643379	0.1095226902
S	0.6377530681	-2.3145267735	-0.358631995
C	-1.0301836625	1.4352979151	0.47902142
C	-1.4770719164	2.3089891499	-0.5266938271
C	-1.3510452732	1.7737424614	1.8066528841
C	-2.2226276742	3.45688446	-0.2285301529
H	-1.2496420951	2.1023184537	-1.5723288714
C	-2.0890657086	2.9200278354	2.1158962066
H	-1.0261486712	1.1322032419	2.6259059801
C	-2.5311809097	3.7668089764	1.096231964
H	-2.5565852032	4.1089970827	-1.0329113459
H	-2.3205442912	3.1516063445	3.1535061553
H	-3.1054876964	4.6588459363	1.3329123061
C	0.4040588262	-3.1927450056	1.2384727048
H	-0.6199255104	-3.1035034323	1.6185070964
H	0.6195145295	-4.2540839683	1.0830727745
H	1.0903730547	-2.817396774	2.005908843
H	-1.5823079851	-0.9401414709	0.5303005691
Si	-2.8531501185	-1.3269007255	-0.2521127994
C	-3.0754036555	-3.1708546241	0.0461344774
H	-3.2126652698	-3.4065696117	1.1070639075
H	-3.9619643814	-3.5304358847	-0.4920445371
C	-4.2257083857	-0.298087355	0.5242325333
H	-4.318244949	-0.4992692295	1.5974493758

H	-5.1894448589	-0.5370904546	0.0561396869
C	-2.6439376877	-0.9631048906	-2.0867167697
H	-3.5531573193	-1.2724806995	-2.6190007862
H	-2.4924128569	0.1027984876	-2.2832487371
H	-2.2036182127	-3.718248706	-0.3252336454
H	-4.0378236949	0.772342131	0.3962855029
H	-1.8019991154	-1.5269119106	-2.5005979421
C	1.5059768825	0.7843848998	-0.774196224
C	1.6886207171	0.7043500398	0.6041887697
C	2.2648970606	0.0904045588	-1.893387378
H	1.0006996767	1.6908624211	-1.1028873638
C	2.6631940616	-0.1570571471	1.3733964119
H	1.3475881481	1.5733460132	1.1652313084
C	3.6437719351	-0.5141400488	-1.5444705879
H	2.4051499282	0.8514095632	-2.6740670275
H	1.6509223109	-0.6943717127	-2.3517850525
C	4.0277804986	0.5497241462	1.5343377523
H	2.7731203484	-1.1372893726	0.9145531721
H	2.257699337	-0.3280052231	2.3796453517
C	4.6315829617	0.4861801398	-0.9841537039
H	3.5022286709	-1.3719527216	-0.8857431297
H	4.0558800949	-0.921424732	-2.4762190095
C	4.7814790908	0.9142921085	0.2764546607
H	3.8800797853	1.4734175013	2.1136902235
H	4.6688201941	-0.082794778	2.1685859812
H	5.3025234731	0.9272630496	-1.7224149465
H	5.5748132627	1.6432466729	0.4496631229

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$TS_{6C\text{-}7B}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.1291980812	0.1181029816	-0.301363147
S	-0.5573864006	2.3008510899	-0.7757007901
C	1.2986157242	-1.3623842435	-0.1605015133
C	1.7720896282	-2.0352061185	-1.300064249
C	1.7553523303	-1.8125088792	1.0900139887
C	2.653050599	-3.1161241305	-1.1962714015
H	1.4571758398	-1.7157994757	-2.2925016172
C	2.6402171301	-2.8912371638	1.2012145541
H	1.4190776027	-1.3242618864	2.0042416085
C	3.0918092274	-3.5491355547	0.0566497485
H	3.0004589747	-3.6172621922	-2.0973709664
H	2.9738785765	-3.2165319003	2.1844422706
H	3.7779057782	-4.3882123814	0.1393251052
C	-1.6850253317	3.2335612294	0.3350033705
H	-1.5963795444	2.9147598569	1.3765403157
H	-1.4376617867	4.2964002517	0.2674773736
H	-2.7197853558	3.0979355963	0.0081572708
H	1.4546861753	0.8628906255	-0.5680698449
Si	1.7687821016	2.3639944183	0.2090015754
C	1.88929543	4.2083226458	-0.2496280505
H	2.7947722037	4.6459600238	0.1924775674
H	1.9582832649	4.3289272563	-1.3369030357
C	1.4108074827	2.1290423818	2.055780444
H	0.4046492864	2.4328212209	2.3600171603
H	2.1266199006	2.7464845532	2.614822441
C	3.5711619247	1.7779372281	-0.0680623421
H	4.2699632241	2.4334536409	0.4700902742
H	3.7119339622	0.7479178369	0.2756584404

H	1.0201890853	4.7819262896	0.0885834461
H	1.5696410253	1.0900082634	2.3637650462
H	3.8412779029	1.8110940648	-1.1309244587
C	-1.5382092325	-1.0892137376	-0.8130251788
C	-1.4955244174	-0.9120607342	0.5553761016
C	-2.4912543862	-0.5148113007	-1.8440786728
H	-0.9814020796	-1.948862193	-1.1811732702
C	-2.415071221	-0.0815228706	1.4201148633
H	-0.9523560798	-1.6777697975	1.108015651
C	-3.8223662663	0.0839531589	-1.3383647685
H	-2.7273420726	-1.3408328232	-2.5291897555
H	-1.9746932671	0.2383211921	-2.4528951102
C	-3.6939256575	-0.8536001443	1.8124067986
H	-2.6778975609	0.8598110115	0.9435729362
H	-1.8852468959	0.1797710425	2.3455236356
C	-4.6890650872	-0.9003941413	-0.5808870325
H	-3.6282510824	0.9863880514	-0.7549260753
H	-4.3767271493	0.4227244894	-2.2221295106
C	-4.6249450493	-1.27934105	0.7022998341
H	-3.4017128191	-1.7559533665	2.3696723677
H	-4.2578626659	-0.2440769722	2.5364162064
H	-5.4592371913	-1.3815386121	-1.1844556253
H	-5.3636711312	-2.0144728316	1.0254857405

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7B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	0.4160294368	-0.2769157019	-0.3420652799
S	0.0922291376	2.0036278465	-0.7505982163
C	1.4340979674	-1.8555676291	-0.1736961194
C	1.7272717194	-2.6681635985	-1.2836994792
C	1.8724393227	-2.3109793817	1.0833471831
C	2.3953451156	-3.8887062486	-1.1434398288
H	1.4362113824	-2.3480334358	-2.2830182088
C	2.5402977997	-3.5305453573	1.2310891277
H	1.6926810802	-1.7078536321	1.9727224853
C	2.8040755746	-4.3291588915	0.1166964957
H	2.6001334358	-4.494808901	-2.0240379345
H	2.8588404118	-3.8545550474	2.2202586748
H	3.3257088032	-5.2766016223	0.2278284204
C	-1.4148765436	2.9893419506	-0.347280522
H	-1.6474873145	2.9729498815	0.7199510542
H	-1.2735983394	4.020133646	-0.6781275496
H	-2.2467253842	2.5550538624	-0.9042998694
H	1.8178917164	0.1788043869	-0.4971599105
Si	1.6772576982	3.0136535246	0.4121430564
C	1.2254951486	4.8489871449	0.4939942107
H	2.0415213205	5.3940044142	0.9858856
H	1.0989559643	5.2799952966	-0.5057497181
C	1.782850976	2.2892383281	2.1502507302
H	0.8252907024	2.3555541036	2.6798451337
H	2.5298124222	2.8339648337	2.7425357908
C	3.2828086732	2.7918153303	-0.5407969254
H	4.103171271	3.2827903711	-0.0009696544
H	3.53213292	1.7334930228	-0.6570349182
H	0.3130011532	5.0405963025	1.068909438
H	2.0808635262	1.2364558195	2.112636139
H	3.2183630097	3.2415712546	-1.5376970716
C	-1.4034056416	-1.2303742408	-0.8241147378

C	-1.3093637227	-1.0682875359	0.543289374
C	-2.3535195788	-0.5480985723	-1.8007341826
H	-0.9798769202	-2.1539928328	-1.2126848489
C	-2.1421868599	-0.1568802289	1.4138950253
H	-0.8563380953	-1.8926313802	1.0924092119
C	-3.7215109329	-0.0696093289	-1.2449924059
H	-2.552637413	-1.2768038006	-2.5968144569
H	-1.8671219656	0.2979292185	-2.3061003518
C	-3.4364746089	-0.8584596318	1.8921445806
H	-2.3824354692	0.7779188772	0.9084161903
H	-1.5647923655	0.1194586534	2.306641753
C	-4.484022749	-1.1128733726	-0.4602827607
H	-3.5915355902	0.8334736868	-0.643438376
H	-4.3293875636	0.2376122701	-2.1057251381
C	-4.3620793762	-1.4227285512	0.8368307219
H	-3.1484288823	-1.6885030667	2.5528580917
H	-3.9979690538	-0.1634373605	2.5373471759
H	-5.2141834873	-1.6837645729	-1.0343485233
H	-5.0231608317	-2.2041851032	1.2140883234

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TS_{6C-8B} B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.1205842548	0.2949049558	-0.0956151255
S	2.1048558474	0.7317741511	0.028836857
C	-2.0879346843	0.2810079777	-0.0748491545
C	-2.8569581085	-0.3180983697	-1.087867391
C	-2.7534558123	0.6825074064	1.0975274942
C	-4.2195660765	-0.57077243	-0.9111874472
H	-2.3867839571	-0.6013762273	-2.0279256394
C	-4.1160547251	0.4341046709	1.2786066859
H	-2.2032121937	1.1912222549	1.887563225
C	-4.8536429177	-0.1992693538	0.2761043059
H	-4.7868196566	-1.0526564352	-1.7039633329
H	-4.6029625749	0.740586238	2.2013628566
H	-5.9148349777	-0.3890122758	0.4130827472
C	2.2164137183	1.8974516903	1.4471974114
H	3.2700949412	2.164508149	1.5724438322
H	1.6501016857	2.8169350079	1.2732705088
H	1.8677166567	1.4488742466	2.3833832838
H	-1.1065727955	1.3131587178	-0.5590890592
Si	0.0477479266	2.1296371349	-1.7063533163
C	-1.6078883988	2.7660295697	-2.4248431529
H	-2.1856444306	3.3447602786	-1.6942520827
H	-1.3979906774	3.4247249763	-3.2785625295
C	0.962352359	3.7046396486	-1.1965708957
H	2.0168277213	3.5220783778	-0.9835461663
H	0.8880771742	4.4191846443	-2.0271730369
C	0.851895857	1.1951718243	-3.1479674693
H	0.8985035622	1.8681490434	-4.0151806555
H	1.862402952	0.8553224583	-2.9104299221
H	-2.2522243004	1.9553687618	-2.7815289813
H	0.2486496768	0.3287035375	-3.4455196292
H	0.5002418029	4.1812704658	-0.3244678426
C	-0.0525420706	-1.5341676628	1.2570078034
C	-0.0047183723	-1.9097348797	-0.058723356
C	1.0110874039	-1.6056782878	2.33084138
H	-1.0526165839	-1.3705258232	1.655365217
C	1.1670213329	-2.4545364979	-0.8412345194

H	-0.9693265097	-2.0610190787	-0.53989288
C	2.2574502261	-2.474945226	2.0576541203
H	0.5050759774	-1.9948217757	3.2264789918
H	1.3428245879	-0.5948975658	2.5957473247
C	1.3055392977	-3.9861323145	-0.6947686539
H	2.094388751	-1.9519476424	-0.5692483819
H	1.0039841918	-2.2384042496	-1.9051484291
C	1.9452961486	-3.9361914337	1.8142501361
H	2.8348861277	-2.032306501	1.2446214097
H	2.8964621879	-2.4042628854	2.9468884652
C	1.5555071603	-4.5435078818	0.6860075076
H	0.3929985856	-4.4608376582	-1.0857121196
H	2.1098644324	-4.3231413886	-1.3677324727
H	2.0362319908	-4.5737967036	2.6944625232
H	1.3892893048	-5.6203099094	0.7478667456

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8B B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.6562480225	-0.7576221229	0.4350101463
S	-0.2290665338	-1.7087852411	2.2921654048
C	1.5077167881	-1.4245889484	2.8350392676
H	1.5843582821	-1.7782491132	3.866704821
H	2.2101864707	-1.9923914913	2.2208948954
H	1.7777738845	-0.3659369558	2.8081212145
Si	0.2979308174	-2.2256024901	-0.9328675098
C	0.7880188668	-1.3867468689	-2.576606092
H	1.5754859496	-0.638421758	-2.4262952609
H	1.1930377693	-2.150810733	-3.2544892199
C	1.8865311007	-3.0640961055	-0.3216235556
H	1.6989048507	-3.6743818151	0.567025211
H	2.2789527596	-3.7182113317	-1.1125860634
C	-0.9848013787	-3.5815343959	-1.2979051921
H	-0.5697256201	-4.300348039	-2.0177613633
H	-1.2447707923	-4.1292813037	-0.3857933336
H	-1.9098459338	-3.1793182191	-1.7261932536
H	2.6722052828	-2.3382856773	-0.081847138
C	-0.9749483921	0.8959372214	-0.6309529067
C	-1.9800870765	-0.0425801669	-0.8816296652
C	-0.9530736187	2.0860245251	0.3171751043
H	-0.2151316363	0.9759501392	-1.408960908
C	-3.3301256327	-0.1950067624	-0.2019539706
H	-1.9289031918	-0.5431302722	-1.84784091
C	-2.2296608755	2.4025950553	1.12376128
H	-0.7056024543	2.9680108322	-0.2918255684
H	-0.109348254	1.9754615542	1.0158951625
C	-4.4166916273	0.7605607507	-0.7343000642
H	-3.2507596278	-0.0963030746	0.8840623162
H	-3.6737103753	-1.2220848834	-0.377517113
C	-3.3707981851	2.9117127067	0.2671621026
H	-2.5143382855	1.5383005582	1.7299596506
H	-1.9697708819	3.1874328619	1.8439880865
C	-4.2426841593	2.2389600655	-0.4945797811
H	-4.5214437791	0.6031396789	-1.818544815
H	-5.3844695028	0.4510177129	-0.3088918576
H	-3.4638396688	3.9980421394	0.2508093985
H	-4.9716176073	2.8431992182	-1.0373810529
H	-0.0456472989	-0.89939353	-3.0940275167

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$TS^{3}_{5A\text{-}11}$ B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	0.517073989078	0.570311474897	-0.383269067530
S	0.281521529752	2.705558804642	-0.585659651076
C	2.035430408530	-0.538260687373	-0.022915187924
C	1.771413705873	3.351369605197	0.286814622624
C	3.212767375452	-0.385189076242	-0.777789497615
C	2.029166993206	-1.530707677027	0.975885569289
H	2.627296579714	2.685920165078	0.155646524278
H	2.008723005190	4.332515521923	-0.130810291171
H	1.561080706511	3.460635472438	1.353887023708
C	4.329478785182	-1.198082144171	-0.563793910359
H	3.266858049231	0.379825394718	-1.551356324857
C	3.141495640333	-2.348249453915	1.195602079661
H	1.142963770601	-1.680782187947	1.589982749551
C	4.294997580064	-2.182480272057	0.425852489543
H	5.225338038293	-1.062050615698	-1.165522638890
H	3.109650662943	-3.111413184189	1.970196830838
H	5.162720335221	-2.814331409333	0.598804155170
C	-1.715987219991	-2.090490549982	0.559557103957
C	-2.101143531665	-1.222216934232	1.505513383835
C	-1.556006432168	-1.915919526991	-0.932236820916
H	-1.467436188124	-3.096793614083	0.898964299589
C	-2.506253204209	0.229496413888	1.359976856505
H	-2.156764335044	-1.611503272509	2.522360653723
C	-2.206178263848	-0.682032425586	-1.596713881828
H	-1.959913849659	-2.816158762303	-1.416011996119
H	-0.479605590039	-1.928377591342	-1.173581358780
C	-3.972495573942	0.437949544585	0.923110822479
H	-1.831196124570	0.767674320815	0.688593815860
H	-2.382640422437	0.721277608807	2.332492166748
C	-3.707461543412	-0.604001341014	-1.433475259047
H	-1.729689884339	0.239189094868	-1.238555502572
H	-1.972163827730	-0.724175125969	-2.667509490436
C	-4.417416345497	-0.145793215115	-0.395556233187
H	-4.625311084739	0.021523205908	1.704294262388
H	-4.183714701193	1.518813513864	0.920709784379
H	-4.274765536653	-0.993898999425	-2.278621026865
H	-5.502692495862	-0.186006075025	-0.500086054361

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11^{3} B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	2.0793445711	-0.9205774134	-0.2174352878
S	2.5876032682	-2.9945040102	-0.5533810645
C	2.2837452551	0.9652180476	0.0089884798
C	2.9765749073	-3.6713135027	1.1161930728
C	2.3089381553	1.5568184549	1.2880749914
C	2.3493343614	1.8389230671	-1.0951881509
H	3.8444479168	-3.1650552239	1.5481747324
H	2.1274332954	-3.5815901279	1.7991964618
H	3.2189930909	-4.7291031003	0.9947204665
C	2.3618883151	2.942013951	1.4601295536
H	2.2847659049	0.9310755132	2.1803916795
C	2.4029458236	3.2255758129	-0.9367292868
H	2.3596668385	1.4383655216	-2.1087161892
C	2.4088129163	3.7808614689	0.3447176079
H	2.3723069337	3.3668461642	2.46135483

H	2.4461664757	3.8723380516	-1.8101020461
H	2.4564229707	4.8593823255	0.4731801497

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$TS^{3}_{11\text{-}23A}$ B3LYP/BSI Optimized geometry (charge = 0, triplet)

Ni	1.3228401979	1.5069321497	0.1095538016
S	0.4906926259	3.424870166	0.669910332
C	2.6227911483	0.1124155137	-0.0142318654
C	-0.4107942382	3.1239226134	2.2487576842
C	3.6620918808	0.166088248	-0.9647203672
C	2.5675750056	-1.0322062877	0.806012907
H	-0.8891001609	4.0617761181	2.5390431805
H	-1.178537914	2.354823439	2.1310677545
H	0.2840014743	2.8296127896	3.040027171
C	4.5778140835	-0.878199532	-1.1151891696
H	3.7708120245	1.0388139021	-1.6089133418
C	3.4790396108	-2.0821602466	0.6655128367
H	1.7943015387	-1.1179890433	1.5683722062
C	4.4872840095	-2.0070172855	-0.2979291979
H	5.3643176316	-0.8094650058	-1.8633283629
H	3.4082956829	-2.9545288586	1.3115793519
H	5.2020206969	-2.819110025	-0.4064261588
S	-1.4126358775	-1.7586761122	1.1607306868
C	-2.6086792311	-0.6561233998	0.3959450089
C	-0.7044257713	-2.5826075874	-0.3201194703
C	-2.1981558116	0.5859238963	-0.1052523188
C	-3.9625978648	-1.0099777252	0.3351309334
H	-1.4807030967	-3.1140367648	-0.8761412149
H	-0.2001325239	-1.8621037267	-0.9684148123
H	0.0349649725	-3.2994579714	0.046708195
C	-3.1236834018	1.4620604709	-0.6714210902
H	-1.1488119486	0.8605687635	-0.0406596856
C	-4.8894969256	-0.1303667914	-0.2291170769
H	-4.2833706906	-1.9683654029	0.7322696673
C	-4.4725544587	1.1032829472	-0.7337782537
H	-2.7904490304	2.4239518336	-1.0510460441
H	-5.938827633	-0.4098265456	-0.2727021703
H	-5.197047005	1.7858814608	-1.1694911166

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$TS_{1\text{-}2}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.4091377593	-0.4250266679	0.4335637675
C	1.4399073466	-0.4762057413	1.107968674
C	1.2151114353	-1.480146729	0.1185116133
C	1.8389618584	-1.6293061082	-1.2729283754
C	3.2407955064	-0.9905354168	-1.4641821606
C	3.1969363545	0.418854114	-2.0118261259
C	2.7373702831	1.537234656	-1.4395230917
C	2.1921309464	1.7994862613	-0.0587404023
C	2.3446480355	0.7543901834	1.0624830127
H	1.3915515943	-0.8590222108	2.1330808629
H	0.9962859727	-2.459911947	0.5546564557
H	1.1815583618	-1.2497106343	-2.0670074284
H	1.9292047885	-2.7067139922	-1.4633226152
H	3.7915939061	-1.0446018659	-0.5187550462
H	3.8049698337	-1.6052408335	-2.1757600124
H	3.5349178174	0.5164338206	-3.0442397827

H	2.7497281035	2.4350190277	-2.0613236007
H	1.1290394847	2.0680855971	-0.1556127584
H	2.6778254927	2.722626461	0.2945154178
H	3.399704774	0.4438002126	1.1119680804
H	2.1668439618	1.2974312456	2.0007663103
C	-1.970796335	-1.5953196099	-0.3282920001
C	-1.3396283709	1.3623954058	1.0145003641
C	-1.7958421003	-0.4907095354	-1.1379280793
C	-2.9561839521	-1.7174887083	0.8163008264
H	-1.5216599007	-2.5333570857	-0.6500009918
C	-1.7845866755	0.3281623794	1.8147063906
C	-2.0285085157	1.8889283826	-0.2285397189
H	-0.5637547445	2.0094918207	1.4201600761
C	-2.6401464698	0.7745242401	-1.1202227027
H	-1.1855638202	-0.6297011869	-2.0306156822
C	-3.0996410033	-0.4208585866	1.6602892151
H	-2.6097907251	-2.5288377332	1.4689377923
H	-3.946463015	-2.030483579	0.4499755831
H	-1.2915956635	0.2070296501	2.7788606549
H	-1.283626191	2.4415621994	-0.8152071583
H	-2.8062023691	2.6230461188	0.0344270266
H	-3.6589805272	0.5441573728	-0.7948996022
H	-2.732828599	1.1541202475	-2.1445685621
H	-3.8576999133	0.2348335134	1.2219865083
H	-3.4748642069	-0.6889707383	2.6549052654

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2 B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.4507227118	-0.250231865	0.377875763
C	1.445112579	-0.0230815463	0.8715505719
C	1.2803248406	-0.9631588214	-0.190085851
C	1.6147397336	-0.7981061504	-1.6662397553
C	3.0960944642	-1.0370959511	-2.0158746154
C	4.1224550577	-0.0742399732	-1.4744636851
C	3.9807847362	1.1066047303	-0.8594352439
C	2.7245030598	1.8532772758	-0.4652589274
C	2.1074233279	1.3558626377	0.8612191025
H	1.5597530124	-0.4970834624	1.8518233632
H	1.3432762941	-2.0128449856	0.1169628826
H	1.2973625431	0.1735570005	-2.0557808099
H	1.027654924	-1.5393805494	-2.2271649526
H	3.3732296981	-2.0472215998	-1.6756357356
H	3.2008968125	-1.0715552389	-3.1134247063
H	5.1484326085	-0.41467785	-1.6290607278
H	4.9050283665	1.5989812281	-0.5531973016
H	1.9730042422	1.8411499682	-1.2597600985
H	2.9900367146	2.9096066524	-0.3282802732
H	2.9146076442	1.3423108207	1.6087192186
H	1.4025382926	2.1212593021	1.2177010042
C	-1.9035845304	-1.6263387389	-0.2197501601
C	-1.5440536892	1.3994865265	1.0371290115
C	-1.958606506	-0.5293273996	-1.0567544386
C	-2.7559051245	-1.8574563356	1.0119692853
H	-1.3639867667	-2.5035628436	-0.5740863564
C	-1.7772773872	0.3381274249	1.8897803039
C	-2.408850798	1.8128155164	-0.137610085
H	-0.8200965617	2.1483332263	1.3561629144
C	-2.9552947244	0.6156015625	-0.9616173848

H	-1.4263205263	-0.6069465975	-2.0045125575
C	-2.9908389384	-0.5779024778	1.8621583187
H	-2.2476130086	-2.6061922411	1.6325741398
H	-3.7255536986	-2.3028404495	0.7395685725
H	-1.1836203409	0.3008299703	2.8026891722
H	-1.7981622587	2.4454557471	-0.7941479961
H	-3.2450088054	2.4472414576	0.1958345151
H	-3.8990696583	0.2610475811	-0.536563777
H	-3.1958779632	0.9643988532	-1.9728125847
H	-3.8659081417	-0.0339746952	1.4942076618
H	-3.2349048119	-0.8781447092	2.8879192228

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$TS_{2\text{-}3}$ B3LYP/BSI Optimized geometry (charge = 0, singlet)

Ni	-0.1237247425	-0.9133561459	-0.388895641
C	-1.9988117315	-1.5193872106	-0.3275684335
C	-1.524753083	-1.1927301584	0.9562353758
C	-1.9188702412	-0.0217245541	1.8541956725
C	-3.3873820176	0.4673458898	1.7164336431
C	-3.5732446015	1.6419902594	0.7790696138
C	-3.2892328933	1.7391980518	-0.5252176465
C	-2.7726463213	0.7127427548	-1.5034478699
C	-2.9920859243	-0.7872498038	-1.2191899753
H	-1.9575325573	-2.5870884969	-0.5660937791
H	-1.1669923166	-2.0535771476	1.5290702431
H	-1.2540138321	0.8401638381	1.716742895
H	-1.7615243668	-0.3513285919	2.888852864
H	-4.0221783927	-0.3807357927	1.4324359638
H	-3.736090421	0.7788866001	2.7077008255
H	-3.9430010747	2.5502059766	1.255629119
H	-3.4476105013	2.7192479934	-0.9785308196
H	-1.6971694428	0.8815106259	-1.6716527555
H	-3.2485012456	0.9353856532	-2.4689181675
H	-4.0164466411	-0.9384418145	-0.8466088701
H	-2.9613499869	-1.2952172759	-2.1916325413
C	1.7832724924	-1.0238615854	-0.8743117298
C	1.2999205012	0.2906268084	-1.0073518533
C	2.7000250307	-1.6324956025	0.1806278004
H	1.8018551274	-1.5943525025	-1.8081545111
C	1.526460927	1.4877214154	-0.0985378974
H	1.0471717898	0.5888204449	-2.0299037481
C	3.3479157931	-0.6759525317	1.2051327424
H	3.5116872605	-2.1516371264	-0.3497954912
H	2.1620228986	-2.4206526517	0.7288049622
C	2.8701722409	2.2042246813	-0.3359589135
H	1.4292978124	1.2218879356	0.9564351092
H	0.7235298281	2.211693313	-0.2914024156
C	4.3454660145	0.2822975642	0.5891673673
H	2.5738305936	-0.152108763	1.7721729539
H	3.8798565958	-1.2953209996	1.9384096941
C	4.1406977822	1.4441150562	-0.0447676464
H	2.909832374	2.5315339787	-1.3863732605
H	2.8800547103	3.1375298267	0.2506572144
H	5.3817934397	-0.0527903606	0.6491035442
H	5.0332001232	1.9511124482	-0.4165306374