Supporting Information

Computational Studies on Ethylene Addition to Nickel Bis(dithiolene)

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Table S1 Bond length(Å) and angles(º) for the examined species at TPSS with different basis sets.

Models	Structural parameters	6-31G**	6-31++ G**	cc-pVDZ	aug-cc-pVDZ	cc-pVTZ	aug-cc-pVTZ	Ave.(*Exp.*[14])
1H	Ni-SX	2.14	2.16	2.17	2.16	2.15	2.15	2.16(2.11)
	SX(')-CX(')	1.72	1.72	1.72	1.72	1.71	1.71	1.72(1.70)
	C1(')-C2(')	1.38	1.38	1.38	1.38	1.37	1.37	1.38(1.37)
	S1(')-Ni-S2(')	92.3	92.3	92.1	92.2	92.0	92.0	92.2(91.5)
	S1(2)-Ni-S1(2)'	87.7	87.7	87.9	87.8	88.0	88.0	87.9(88.5)
	Ni-SX(')-CX(')	104.0	103.5	103.5	103.5	103.7	103.8	103.7(103.9)
	SX(')-CX(')-CY(')	119.9	120.3	120.5	120.4	120.3	120.2	120.3(120.2)
TS_{2yH}	Ni-S1(')	2.16	2.17	2.18	2.18	2.17	2.17	2.17
	Ni-S2(')	2.09	2.12	2.13	2.12	2.11	2.11	2.11
	S1(')-C1(')	1.74	1.74	1.74	1.74	1.74	1.74	1.74
	S2(')-C2(')	1.75	1.75	1.75	1.75	1.73	1.74	1.74
	C1(')-C2(')	1.37	1.37	1.37	1.37	1.36	1.36	1.37
	S1(')-Ni-S2(')	92.3	92.2	92.0	91.9	91.5	91.5	91.9
	Ni-S2(')-C2(')	106.0	105.2	105.0	105.3	105.8	105.8	105.5
	Ni-S1(')-C1(')	101.9	101.7	101.6	101.8	102.2	102.2	101.9
	S2(')-C2(')-C1(')	115.7	116.4	116.5	116.5	116.3	116.3	116.3
	S1(')-C1(')-C2(')	122.3	122.6	122.9	122.7	122.5	122.5	122.6
	S2-C3	2.27	2.30	2.30	2.31	2.30	2.30	2.30
	S2'-C4	2.27	2.30	2.30	2.31	2.30	2.30	2.30
	C3-C4	1.43	1.43	1.43	1.43	1.42	1.42	1.43
2yH	Ni-S1(')	2.17	2.19	2.20	2.20	2.19	2.19	2.19
	Ni-S2(')	2.11	2.15	2.16	2.15	2.13	2.13	2.14
	S1(')-C1(')	1.77	1.77	1.78	1.77	1.77	1.77	1.77
	S2(')-C2(')	1.75	1.75	1.75	1.75	1.74	1.74	1.74
	C1(')-C2(')	1.36	1.36	1.36	1.36	1.35	1.35	1.36
	S1(')-Ni-S2(')	91.3	91.2	90.8	90.8	90.4	90.4	90.8
	Ni-S2(')-C2(')	105.7	104.6	104.3	104.7	105.4	105.4	105.0
	Ni-S1(')-C1(')	100.8	100.6	100.5	100.7	101.0	101.0	100.8
	S2(')-C2(')-C1(')	113.0	113.5	113.5	113.4	113.2	113.2	113.3
	S1(')-C1(')-C2(')	124.5	124.9	125.2	124.9	124.8	124.8	124.9

	S2-C3	1.88	1.88	1.88	1.88	1.87	1.87	1.88
	S2’-C4	1.88	1.88	1.88	1.88	1.87	1.87	1.88
	C3-C4	1.53	1.53	1.53	1.53	1.53	1.53	1.53
2H	Ni-S1	2.21	2.18	2.20	2.20	2.18	2.18	2.19
	Ni-S2	2.27	2.23	2.24	2.23	2.21	2.21	2.23
	Ni-S1’	2.21	2.19	2.20	2.19	2.18	2.18	2.19
	Ni-S2’	2.25	2.21	2.23	2.21	2.20	2.19	2.22
	S1-C1	1.74	1.74	1.74	1.74	1.73	1.73	1.74
	S2-C2	1.77	1.77	1.77	1.78	1.76	1.77	1.77
	S1’-C1’	1.75	1.74	1.75	1.75	1.74	1.74	1.75
	S2’-C2’	1.77	1.78	1.78	1.78	1.77	1.77	1.78
	C1-C2	1.36	1.36	1.36	1.36	1.35	1.35	1.36
	C1’-C2’	1.35	1.36	1.36	1.36	1.35	1.35	1.36
	S1-Ni-S2	91.7	92.0	91.9	92.0	91.8	91.8	91.9
	S1’-Ni-S2’	91.5	91.9	91.6	91.7	91.4	91.4	91.6
	Ni-S1-C1	101.2	101.1	101.9	101.1	101.2	101.2	101.3
	Ni-S2-C2	103.3	102.4	102.1	102.5	102.9	102.9	102.7
	Ni-S1’-C1’	101.8	101.3	101.1	101.2	101.3	101.4	101.4
	Ni-S2’-C2’	104.6	103.0	102.6	102.9	103.4	103.4	103.3
	S1-C1-C2	125.1	125.4	125.7	125.5	125.4	125.4	125.4
	S1’-C1’-C2’	124.5	125.3	125.6	125.3	125.3	125.2	125.2
	S2-C2-C1	115.8	116.9	116.9	116.9	116.6	116.6	116.6
	S2’-C2’-C1’	114.8	115.9	116.0	115.9	115.6	115.6	115.6
	S2-C3	1.87	1.88	1.88	1.88	1.87	1.87	1.88
	S2’-C4	1.87	1.88	1.89	1.89	1.88	1.88	1.88
	C3-C4	1.53	1.54	1.53	1.54	1.53	1.53	1.53
TS_{3H}	Ni-S1(2)	2.15	2.18	2.19	2.19	2.17	2.17	2.18
	Ni-S1(2)’	2.13	2.15	2.16	2.16	2.14	2.14	2.15
	S1(2)-C1(2)	1.77	1.77	1.77	1.77	1.76	1.76	1.76
	S1(2)’-C1(2)’	1.74	1.74	1.75	1.75	1.74	1.74	1.74
	C1-C2	1.35	1.35	1.35	1.35	1.34	1.34	1.35
	C1’-C2’	1.36	1.36	1.36	1.36	1.35	1.35	1.35
	S1-Ni-S2	86.2	86.6	86.3	86.4	86.2	86.2	86.3
	S1’-Ni-S2’	92.4	92.4	92.3	92.4	92.1	92.1	92.3
	Ni-S1(2)-C1(2)	101.9	101.4	101.3	101.7	101.9	101.9	101.7
	Ni-S1(2)’-C1(2)’	104.2	103.9	103.8	103.8	104.0	104.1	104.0
	S1-C1-C2	116.8	117.6	117.7	117.6	117.5	117.5	117.5

	S2-C2-C1	116.8	117.6	117.7	117.6	117.5	117.5	117.5
	S1'-C1'-C2'	119.5	119.9	120.1	120.0	119.9	119.9	119.9
	S2'-C2'-C1'	119.5	119.9	120.1	120.0	119.9	119.9	119.9
	S1(2)-C3(4)	2.22	2.25	2.24	2.25	2.25	2.25	2.24
	C3-C4	1.44	1.44	1.44	1.44	1.43	1.43	1.44
3H	Ni-S1(2)	2.19	2.23	2.25	2.23	2.22	2.22	2.22
	Ni-S1(2)'	2.19	2.23	2.25	2.23	2.22	2.22	2.22
	S1(2)-C1(2)	1.81	1.81	1.81	1.81	1.80	1.80	1.81
	S1(2)'-C1(2)'	1.76	1.76	1.76	1.76	1.75	1.75	1.76
	C1-C2	1.34	1.34	1.34	1.34	1.33	1.33	1.34
	C1'-C2'	1.35	1.35	1.35	1.35	1.34	1.34	1.35
	S1-Ni-S2	83.1	83.1	82.8	83.0	82.6	82.7	82.9
	S1'-Ni-S2'	92.4	92.2	92.0	92.2	91.7	91.7	92.0
	Ni-S1(2)-C1(2)	99.2	98.1	98.0	98.3	98.6	98.5	98.5
	Ni-S1(2)'-C1(2)'	104.6	104.5	104.4	104.3	104.8	104.8	104.6
	S1-C1-C2	115.6	116.5	116.7	116.5	116.4	116.4	116.4
	S2-C2-C1	115.6	116.5	116.7	116.5	116.4	116.4	116.4
	S1'-C1'-C2'	119.2	119.4	119.6	119.6	119.4	119.4	119.4
	S2'-C2'-C1'	119.2	119.4	119.6	119.6	119.4	119.4	119.4
	S1(2)-C3(4)	1.90	1.89	1.90	1.90	1.88	1.88	1.89
	C3-C4	1.53	1.54	1.53	1.53	1.53	1.53	1.53
4H	Ni-S1	2.24	2.24	2.26	2.25	2.24	2.24	2.24
	Ni-S2	2.22	2.23	2.24	2.24	2.23	2.23	2.23
	Ni-S1'	2.22	2.23	2.24	2.24	2.23	2.23	2.23
	Ni-S2'	2.24	2.24	2.26	2.25	2.24	2.24	2.24
	S1-C1	1.73	1.73	1.73	1.73	1.72	1.72	1.73
	S2-C2	1.73	1.73	1.73	1.73	1.72	1.72	1.73
	S1'-C1'	1.73	1.73	1.73	1.74	1.72	1.72	1.73
	S2'-C2'	1.73	1.73	1.73	1.74	1.72	1.72	1.73
	C1(')-C2(')	1.37	1.37	1.37	1.37	1.36	1.36	1.37
	S1(')-Ni-S2(')	89.9	90.0	89.8	89.7	89.4	89.4	89.7
	Ni-S1-C1	102.9	102.8	102.7	102.9	103.2	103.2	103.0
	Ni-S2-C2	103.1	103.0	102.9	103.1	103.3	103.4	103.1
	Ni-S1'-C1'	103.1	103.0	102.9	103.1	103.3	103.4	103.1
	Ni-S2'-C2'	102.9	102.8	102.7	102.9	103.2	103.2	103.0
	S1-C1-C2	121.1	121.3	121.4	121.3	121.2	121.2	121.3
	S2-C2-C1	120.9	121.0	121.2	121.0	121.0	121.0	121.0

	S1’-C1’-C2’	120.9	121.0	121.2	121.0	121.0	121.0	121.0
	S2’-C2’-C1’	121.1	121.3	121.4	121.3	121.2	121.2	121.3
	Ni-C3(4)	2.00	2.07	2.08	2.08	2.08	2.08	2.06
	C3-C4	1.41	1.41	1.40	1.41	1.40	1.40	1.40
5H	Ni-S1	2.24	2.24	2.25	2.25	2.24	2.24	2.24
	Ni-S2	2.29	2.27	2.28	2.27	2.26	2.26	2.27
	Ni-S1’	2.15	2.16	2.17	2.17	2.16	2.16	2.16
	Ni-S2’	2.18	2.19	2.20	2.20	2.18	2.18	2.19
	S1-C1	1.74	1.73	1.74	1.74	1.73	1.73	1.74
	S2-C2	1.77	1.77	1.77	1.77	1.76	1.76	1.77
	S1’-C1’	1.74	1.74	1.75	1.75	1.74	1.74	1.74
	S2’-C2’	1.74	1.74	1.75	1.75	1.74	1.74	1.74
	C1(’)-C2(’)	1.36	1.36	1.36	1.36	1.35	1.35	1.35
	S1-Ni-S2	91.0	91.3	91.2	91.2	91.0	91.0	91.1
	S1’-Ni-S2’	91.6	91.8	91.6	91.6	91.2	91.2	91.5
	Ni-S1-C1	101.2	101.4	101.2	101.4	101.5	101.6	101.4
	Ni-S2-C2	101.4	102.3	102.4	102.3	102.5	102.6	102.3
	Ni-S1’-C1’	103.9	103.4	103.4	103.5	103.8	103.8	103.6
	Ni-S2’-C2’	103.4	102.8	102.7	102.8	103.1	103.1	103.0
	S1-C1-C2	125.5	125.3	125.6	125.3	125.3	125.3	125.4
	S2-C2-C1	119.1	119.1	119.3	119.1	119.1	119.1	119.1
	S1’-C1’-C2’	120.3	120.6	120.7	120.6	120.5	120.5	120.5
	S2’-C2’-C1’	119.7	120.1	120.2	120.1	120.0	120.0	120.0
	S2-C3	1.89	1.92	1.92	1.92	1.91	1.91	1.91
	Ni-C4	1.94	1.99	2.00	2.00	2.00	2.00	1.98
	C3-C4	1.51	1.50	1.50	1.50	1.50	1.50	1.50

Table S2 Bond length(Å) and angles(º) for the examined speices with different density functionals based on 6-31++G** basis set.

Models	Structural parameters	B3LYP (HFE = 20%)	B3PW91 (HFE = 20%)	BMK (HFE = 42%)	HSE06 (HFE = 25%)	LC- ω PBE (HFE = 25%)	M05 (HFE = 28%)	M06 (HFE = 27%)	O3LYP (HFE = 20%)	ω-B97X (HFE= 100% for long-range) (HFE =20% for short-range)	ω-B97XD (HFE= 100% for long-range) (HFE =20% for short-range)	Ave. (*Exp.*[14])
1H	Ni-SX	2.17	2.15	2.18	2.15	2.11	2.15	2.16	2.16	2.13	2.15	2.15(2.11)
	SX(')-CX(')	1.71	1.70	1.71	1.70	1.70	1.70	1.70	1.70	1.69	1.70	1.70(1.70)
	C1(')-C2(')	1.38	1.38	1.38	1.38	1.37	1.38	1.37	1.38	1.37	1.37	1.38(1.37)
	S1(')-Ni-S2(')	92.2	92.5	92.9	92.6	92.8	92.7	92.8	92.0	92.7	92.7	92.6(91.5)
	S1(2)-Ni-S1(2)'	87.8	87.5	87.1	87.4	87.2	87.3	87.2	88.0	87.3	87.3	87.4(88.5)
	Ni-SX(')-CX(')	102.9	103.2	102.4	103.0	103.7	102.9	102.6	103.4	103.2	103.0	103.7(103.9)
	SX(')-CX(')-CY(')	120.9	120.6	121.2	120.7	120.0	120.8	121.0	120.6	120.5	120.7	120.3(120.2)
TS_{2yH}	Ni-S1(')	2.19	2.16	2.19	2.16	2.13	2.16	2.17	2.17	2.15	2.16	2.16
	Ni-S2(')	2.14	2.11	2.15	2.11	2.07	2.11	2.12	2.12	2.10	2.11	2.11
	S1(')-C1(')	1.73	1.72	1.73	1.72	1.71	1.72	1.72	1.72	1.72	1.72	1.72
	S2(')-C2(')	1.74	1.73	1.75	1.72	1.71	1.72	1.73	1.73	1.72	1.72	1.72
	C1(')-C2(')	1.36	1.36	1.36	1.36	1.35	1.36	1.36	1.37	1.36	1.36	1.36
	S1(')-Ni-S2(')	92.0	92.2	92.1	92.2	92.3	92.1	92.3	91.9	92.2	92.2	92.2
	Ni-S2(')-C2(')	104.4	104.9	104.3	104.8	105.6	104.6	104.3	105.0	104.9	104.8	104.8
	Ni-S1(')-C1(')	101.3	101.7	101.5	101.7	102.4	101.6	101.2	101.8	101.8	101.7	101.7
	S2(')-C2(')-C1(')	117.4	117.2	117.9	117.3	116.9	117.4	117.4	117.1	117.3	117.5	117.3
	S1(')-C1(')-C2(')	123.1	122.5	122.8	122.5	121.6	122.4	123.0	122.6	122.3	122.4	122.5
	S2-C3	2.36	2.37	2.44	2.38	2.45	2.46	2.38	2.35	2.43	2.42	2.39
	S2'-C4	2.36	2.37	2.44	2.38	2.45	2.32	2.38	2.35	2.43	2.42	2.38
	C3-C4	1.42	1.40	1.40	1.40	1.38	1.40	1.40	1.41	1.39	1.39	1.40
2yH	Ni-S1(')	2.21	2.19	2.22	2.18	2.16	2.19	2.19	2.19	2.19	2.19	2.19
	Ni-S2(')	2.19	2.16	2.22	2.16	2.13	2.16	2.17	2.15	2.18	2.18	2.17
	S1(')-C1(')	1.75	1.74	1.76	1.74	1.73	1.73	1.74	1.74	1.74	1.74	1.74
	S2(')-C2(')	1.77	1.76	1.79	1.76	1.75	1.76	1.77	1.76	1.76	1.76	1.76
	C1(')-C2(')	1.35	1.35	1.35	1.35	1.34	1.36	1.34	1.36	1.35	1.35	1.35
	S1(')-Ni-S2(')	90.7	90.8	90.5	90.8	90.7	90.6	90.9	90.7	90.6	90.6	90.7
	Ni-S2(')-C2(')	103.2	103.9	102.2	103.8	104.0	103.7	102.8	104.3	103.2	103.2	103.4
	Ni-S1(')-C1(')	99.8	100.1	99.4	100.0	100.1	99.9	99.4	100.3	99.8	99.8	99.8

	S2(')-C2(')-C1(')	114.4	113.8	114.4	113.8	113.5	113.6	114.0	113.8	114.2	114.2	114.0
	S1(')-C1(')-C2(')	125.8	125.4	126.2	125.5	125.1	125.6	125.9	125.3	125.6	125.6	125.6
	S2-C3	1.86	1.85	1.87	1.84	1.82	1.85	1.85	1.85	1.84	1.84	1.85
	S2'-C4	1.86	1.85	1.87	1.84	1.82	1.85	1.85	1.85	1.84	1.84	1.85
	C3-C4	1.53	1.53	1.54	1.52	1.53	1.52	1.52	1.53	1.53	1.53	1.53
2H	Ni-S1	2.21	2.18	2.21	2.18	2.16	2.19	2.19	2.19	2.19	2.18	2.19
	Ni-S2	2.26	2.23	2.27	2.23	2.20	2.23	2.25	2.23	2.24	2.24	2.24
	Ni-S1'	2.21	2.18	2.21	2.18	2.16	2.19	2.19	2.19	2.19	2.18	2.19
	Ni-S2'	2.25	2.22	2.26	2.22	2.19	2.22	2.24	2.22	2.23	2.23	2.23
	S1-C1	1.74	1.73	1.75	1.73	1.72	1.72	1.73	1.73	1.73	1.73	1.73
	S2-C2	1.77	1.76	1.79	1.76	1.75	1.76	1.77	1.76	1.76	1.76	1.76
	S1'-C1'	1.74	1.73	1.75	1.73	1.73	1.73	1.73	1.73	1.73	1.74	1.73
	S2'-C2'	1.77	1.77	1.79	1.76	1.76	1.77	1.77	1.77	1.76	1.77	1.77
	C1-C2	1.35	1.35	1.35	1.35	1.34	1.35	1.35	1.36	1.34	1.35	1.35
	C1'-C2'	1.35	1.35	1.35	1.35	1.34	1.35	1.35	1.35	1.35	1.34	1.35
	S1-Ni-S2	91.7	91.9	92.1	92.0	92.1	92.0	92.2	91.7	91.9	91.9	91.9
	S1'-Ni-S2'	91.5	91.7	91.8	91.8	91.8	91.7	92.1	91.4	91.8	91.7	91.7
	Ni-S1-C1	100.6	100.8	100.5	100.7	101.1	100.6	100.4	100.9	100.8	100.8	100.7
	Ni-S2-C2	101.5	102.1	101.4	101.9	102.6	101.8	101.3	101.3	101.8	101.9	101.8
	Ni-S1'-C1'	100.6	100.8	100.5	100.8	101.0	100.5	100.3	101.0	100.7	100.7	100.7
	Ni-S2'-C2'	101.7	102.3	101.5	102.1	102.7	101.9	101.3	101.5	101.8	101.9	101.9
	S1-C1-C2	126.3	125.8	126.4	125.9	125.4	126.1	126.3	125.8	125.9	125.9	126.0
	S1'-C1'-C2'	126.2	125.8	126.3	125.8	125.3	126.0	126.2	125.7	125.9	125.9	125.9
	S2-C2-C1	117.3	117.2	117.5	117.3	116.8	117.2	117.6	117.1	117.4	117.4	117.3
	S2'-C2'-C1'	117.0	116.4	116.8	116.5	116.1	116.3	116.9	116.3	116.8	116.9	116.9
	S2-C3	1.87	1.85	1.87	1.84	1.82	1.85	1.86	1.86	1.84	1.83	1.86
	S2'-C4	1.87	1.86	1.88	1.85	1.83	1.86	1.86	1.86	1.85	1.84	1.86
	C3-C4	1.53	1.53	1.54	1.53	1.53	1.52	1.52	1.53	1.53	1.53	1.53
TS_{3H}	Ni-S1(2)	2.21	2.17	2.20	2.17	2.13	2.17	2.18	2.18	2.17	2.18	2.18
	Ni-S1(2)'	2.16	2.14	2.17	2.14	2.11	2.15	2.15	2.15	2.13	2.14	2.14
	S1(2)-C1(2)	1.75	1.74	1.75	1.73	1.70	1.73	1.74	1.75	1.71	1.72	1.73
	S1(2)'-C1(2)'	1.74	1.73	1.75	1.72	1.73	1.73	1.73	1.73	1.73	1.73	1.73
	C1-C2	1.35	1.35	1.36	1.35	1.36	1.35	1.35	1.35	1.36	1.36	1.35
	C1'-C2'	1.36	1.36	1.36	1.36	1.34	1.36	1.35	1.36	1.34	1.35	1.35
	S1-Ni-S2	86.6	87.8	87.8	87.6	88.4	87.5	87.8	86.6	87.6	87.7	87.5
	S1'-Ni-S2'	92.6	92.7	93.6	92.9	92.7	92.7	93.0	92.1	92.9	92.9	92.8
	Ni-S1(2)-C1(2)	100.8	101.5	101.3	101.6	103.2	101.6	101.5	101.4	102.5	102.3	101.8

	Ni-S1(2)'-C1(2)'	103.0	103.2	102.0	103.0	103.8	103.2	102.8	103.7	103.3	103.0	103.1
	S1-C1-C2	118.6	118.3	119.1	118.4	118.4	118.5	118.9	118.1	118.9	118.8	118.6
	S2-C2-C1	118.6	118.3	119.1	118.4	118.4	118.5	118.9	118.1	118.9	118.8	118.6
	S1'-C1'-C2'	120.7	120.3	121.1	120.5	119.7	120.4	120.7	120.2	120.3	120.5	120.4
	S2'-C2'-C1'	120.7	120.3	121.1	120.5	119.7	120.4	120.7	120.2	120.3	120.5	120.4
	S1(2)-C3(4)	2.32	2.34	2.42	2.34	2.44	2.36	2.35	2.31	2.42	2.40	2.36
	C3-C4	1.42	1.41	1.40	1.41	1.38	1.41	1.40	1.42	1.39	1.40	1.41
3H	Ni-S1(2)	2.30	2.25	2.29	2.25	2.24	2.27	2.27	2.26	2.28	2.28	2.27
	Ni-S1(2)'	2.15	2.13	2.16	2.13	2.11	2.13	2.14	2.14	2.13	2.14	2.14
	S1(2)-C1(2)	1.79	1.79	1.81	1.79	1.78	1.78	1.79	1.79	1.78	1.79	1.79
	S1(2)'-C1(2)'	1.76	1.75	1.78	1.75	1.74	1.75	1.75	1.75	1.75	1.75	1.75
	C1-C2	1.34	1.33	1.34	1.33	1.33	1.34	1.33	1.34	1.33	1.33	1.33
	C1'-C2'	1.34	1.34	1.34	1.34	1.33	1.34	1.34	1.34	1.34	1.34	1.34
	S1-Ni-S2	81.5	82.3	82.1	82.3	82.3	82.0	82.6	81.7	81.4	81.7	82.0
	S1'-Ni-S2'	92.4	92.4	93.5	92.6	92.3	92.2	92.6	91.8	92.6	92.6	92.5
	Ni-S1(2)-C1(2)	96.9	97.2	97.3	97.2	97.2	97.0	97.3	97.3	96.8	97.3	97.2
	Ni-S1(2)'-C1(2)'	103.7	103.0	102.8	103.8	104.5	104.3	103.7	104.5	104.8	103.6	103.9
	S1-C1-C2	117.6	117.1	117.5	117.1	117.0	117.4	117.7	117.0	117.5	117.5	117.3
	S2-C2-C1	117.6	117.1	117.5	117.1	117.0	117.4	117.7	117.0	117.5	117.5	117.3
	S1'-C1'-C2'	120.7	119.8	120.5	119.9	119.4	119.6	120.0	119.6	119.9	120.0	119.9
	S2'-C2'-C1'	120.7	119.8	120.5	119.9	119.4	119.6	120.0	119.6	119.9	120.0	119.9
	S1(2)-C3(4)	1.87	1.86	1.88	1.85	1.82	1.85	1.86	1.86	1.84	1.85	1.86
	C3-C4	1.54	1.53	1.54	1.53	1.53	1.53	1.53	1.53	1.54	1.54	1.53
5H	Ni-S1	2.26	2.23	2.23	2.22	2.18	2.23	2.23	2.24	2.21	2.22	2.23
	Ni-S2	2.26	2.22	2.21	2.21	2.15	2.22	2.22	2.23	2.17	2.20	2.21
	Ni-S1'	2.26	2.22	2.21	2.21	2.15	2.22	2.22	2.23	2.17	2.20	2.21
	Ni-S2'	2.26	2.23	2.23	2.22	2.18	2.23	2.23	2.24	2.21	2.22	2.23
	S1-C1	1.73	1.72	1.74	1.72	1.72	1.72	1.72	1.72	1.72	1.72	1.72
	S2-C2	1.72	1.72	1.75	1.71	1.72	1.72	1.72	1.72	1.72	1.72	1.72
	S1'-C1'	1.72	1.72	1.75	1.71	1.72	1.72	1.72	1.72	1.72	1.72	1.72
	S2'-C2'	1.73	1.72	1.74	1.72	1.72	1.72	1.72	1.72	1.72	1.72	1.72
	C1(')-C2(')	1.37	1.36	1.36	1.36	1.34	1.36	1.36	1.37	1.35	1.35	1.36
	S1(')-Ni-S2(')	89.7	90.0	90.4	90.1	90.4	89.9	90.2	89.4	90.2	90.0	90.0
	Ni-S1-C1	102.6	102.8	102.7	102.7	103.1	102.7	102.3	103.1	102.8	102.8	102.8
	Ni-S2-C2	102.5	102.9	103.2	102.8	104.0	102.8	102.4	103.2	103.5	103.3	103.1
	Ni-S1'-C1'	102.5	102.9	103.2	102.8	104.0	102.8	102.4	103.2	103.5	103.3	103.1
	Ni-S2'-C2'	102.6	102.8	102.7	102.7	103.1	102.7	102.3	103.1	102.8	102.8	102.8

	S1-C1-C2	121.8	121.3	121.3	121.3	120.7	121.4	121.7	121.3	121.1	121.2	121.3
	S2-C2-C1	121.5	121.0	120.6	121.0	119.8	121.1	121.4	121.1	120.4	120.7	120.9
	S1'-C1'-C2'	121.5	121.0	120.6	121.0	119.8	121.1	121.4	121.1	120.4	120.7	120.9
	S2'-C2'-C1'	121.8	121.3	121.3	121.3	120.7	121.4	121.7	121.3	121.1	121.2	121.3
	Ni-C3(4)	2.13	2.08	2.09	2.08	2.02	2.07	2.10	2.09	2.08	2.10	2.08
	C3-C4	1.38	1.39	1.40	1.39	1.41	1.39	1.39	1.39	1.40	1.39	1.39
4H	Ni-S1	2.26	2.23	2.24	2.23	2.20	2.24	2.24	2.24	2.22	2.23	2.23
	Ni-S2	2.30	2.26	2.27	2.26	2.22	2.26	2.27	2.27	2.26	2.26	2.26
	Ni-S1'	2.17	2.14	2.15	2.14	2.11	2.15	2.15	2.16	2.13	2.14	2.15
	Ni-S2'	2.20	2.18	2.19	2.17	2.14	2.18	2.19	2.19	2.16	2.17	2.18
	S1-C1	1.73	1.72	1.75	1.72	1.72	1.72	1.73	1.72	1.73	1.73	1.73
	S2-C2	1.77	1.76	1.79	1.75	1.75	1.76	1.76	1.76	1.76	1.76	1.76
	S1'-C1'	1.74	1.73	1.76	1.73	1.73	1.73	1.74	1.73	1.74	1.74	1.74
	S2'-C2'	1.74	1.73	1.76	1.73	1.73	1.73	1.74	1.73	1.74	1.74	1.74
	C1(')-C2(')	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.35	1.34	1.35	1.35
	S1-Ni-S2	90.9	91.3	91.8	91.5	91.8	91.5	91.7	91.3	91.5	91.5	91.5
	S1'-Ni-S2'	91.8	92.0	92.7	92.1	92.6	91.9	92.3	91.8	92.5	92.3	92.2
	Ni-S1-C1	101.2	101.3	101.4	101.2	101.3	100.9	100.5	101.4	101.2	101.1	101.2
	Ni-S2-C2	101.9	102.2	102.0	102.1	102.4	102.0	101.4	102.4	102.0	102.0	102.0
	Ni-S1'-C1'	103.0	103.2	102.6	103.0	103.2	103.2	102.5	103.6	102.8	102.8	103.0
	Ni-S2'-C2'	102.3	102.5	101.8	102.3	102.6	102.4	101.9	102.9	102.2	102.1	102.3
	S1-C1-C2	125.9	125.6	125.5	125.6	125.7	125.8	126.1	125.6	125.5	125.6	125.7
	S2-C2-C1	119.7	119.2	120.0	119.2	118.7	119.2	119.5	119.3	119.2	119.2	119.3
	S1'-C1'-C2'	121.0	121.7	119.9	120.7	120.4	120.7	121.0	120.6	120.7	120.8	120.8
	S2'-C2'-C1'	120.5	121.2	120.3	120.2	119.7	120.3	120.5	120.1	120.1	120.2	120.3
	S2-C3	1.90	1.88	1.91	1.88	1.84	1.88	1.89	1.92	1.86	1.88	1.89
	Ni-C4	2.00	1.98	1.96	1.97	1.94	1.98	1.98	1.99	1.96	1.97	1.97
	C3-C4	1.50	1.50	1.51	1.50	1.50	1.49	1.49	1.50	1.51	1.50	1.50

Table S3 Bond length(Å) and angles(º) for nickel dithiolenes from experimental measurements and the average values for **1H** from calculations with different density functionals based on 6-31++G** basis set in current work.

Structural Parameters	Exp.					Ave. in Calc.
	$Ni(S_2C_2H_2)_2$	$Ni(S_2C_2Me_2)_2$	$Ni(S_2C_2Ph_2)_2$	$Ni[S_2C_2(CF_3)_2]_2$	Ave.	$Ni(S_2C_2H_2)_2$
Ni-SX		2.13	2.10	2.11	2.11	2.15
SX-CX	1.69	1.71	1.69 (1.72)	1.69	1.70	1.70
CX-CY	1.36	1.37	1.37	1.38	1.37	1.38
S1(')-Ni-S2(')	92.6	91.4	89.8	92.1	91.5	92.6
S1(2)-Ni-S1(2)'	87.4		90.2	87.9	88.5	87.4
SX-CX-CY	120.2				120.2	120.3
Ni-SX-CX	103.9				103.9	103.7

Complete Reference for Ref (14):

The calculated average values of Ni-S, C-S, C-C bond lengthes and S-Ni-S, S-C-C and Ni-S-C angles in **1H** are compared with the corresponding bond lengthes and angles in $Ni(S_2C_2H_2)_2$[S1], $Ni(S_2C_2Me_2)_2$[S2], $Ni(S_2C_2Ph_2)_2$[S3] and $Ni[S_2C_2(CF_3)_2]_2$[S4] from the experimental measurement in Table S1, no large differences are found.

Complete Reference for Ref (19):

Gaussian 09, Revision **A.1**, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, Jr., J. A.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, N. J.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Table S4 The computated energies of the spin-purified low-spin (LS) from the broken-spin-symmetry (BS) energies, triplet state (HS) energies and their total spin operator $<S^2>$ for the species whose singlet states are not pure according to stability analysis. The energies are in a.u..

Methods	B3LYP	B3 PW91	BMK	HSE06	LC-ωPBE	M05	M06	O3LYP	TPSS	ω-B97X	ω-B97XD
Species			**1H**		**1H**					**1H**	**1H**
^{BS}E			-3254.4944		-3254.95079					-3255.7095	-3255.7090
$^{BS}<S^2>$			0.526		0.7339					0.7262	0.599
^{HS}E			-3254.4570		-3254.94274					-3255.6731	-3255.6995
$^{HS}<S^2>$			2.037		2.0391					2.0266	2.0166
^{LS}E			-3254.5074		-3254.95526					-3255.7299	-3255.7130
Species	**4H**	**4H**	**4H**	**4H**	**4H**	**4H**	**4H**	**4H**	**4H**	**4H**	**4H**
^{BS}E	-3334.4408	-3334.1129	-3332.9960	-3333.3575	-3333.4675	-3334.2305	-3334.0506	-3334.5057	-3334.5772	-3334.2544	-3334.2440
$^{BS}<S^2>$	0.9254	0.8664	0.8647	0.8836	0.8556	0.8465	0.8527	0.8238	0.6067	0.9409	0.9293
^{HS}E	-3334.45086	-3334.12084	-3333.0167	-3333.3663	-3333.4857	-3334.2427	-3334.0595	-3334.5132	-3334.5798	-3334.2507	-3334.2566
$^{HS}<S^2>$	2.0207	2.0206	2.014	2.029	2.0651	2.0061	2.0128	2.0124	2.0069	2.0156	2.0139
^{LS}E	-3334.4323	-3334.1070	-3332.9804	-3333.3507	-3333.4546	-3334.2216	-3334.0432	-3334.5005	-3334.5761	-3334.2576	-3334.2331

Cartesian coordinates for all the complexes calculated in this study:

TPSS/6-31G**

1H

E = -3255.896747 au

Ni	0.000000	0.000102	0.000000
S	-0.000432	-0.000078	2.139754
S	2.138046	-0.000073	-0.085474
S	-2.138046	-0.000654	0.085474
S	0.000432	-0.000641	-2.139754
C	1.666488	-0.000021	2.555409
C	2.619623	-0.000019	1.563609
C	-2.619623	-0.001170	-1.563609
C	-1.666488	-0.001164	-2.555409
H	1.923023	0.000026	3.613383
H	3.686957	0.000030	1.777893
H	-3.686956	-0.001479	-1.777893
H	-1.923022	-0.001467	-3.613383

TS_{2yH}

E = -3334.469686 au

Ni	0.019989	0.014070	-0.021855
S	-0.022385	0.040538	2.065507
S	2.173635	-0.076807	-0.062450
S	-1.651527	-1.218832	-0.235309
S	-0.547554	1.221433	-1.715452
C	1.594756	-0.378995	2.585849
C	2.553324	-0.356981	1.613593
C	-2.709088	-0.405402	-1.367476
C	-2.153620	0.638339	-2.050616
C	-1.612566	-1.398336	2.814579
C	-2.604716	-1.570278	1.796454
H	-1.001516	-2.259306	3.079898
H	-1.851202	-0.735284	3.641801
H	-3.427655	-0.858461	1.762807
H	-2.868773	-2.587184	1.518858
H	1.795246	-0.493414	3.648087
H	3.608513	-0.473445	1.859573
H	-3.683629	-0.835851	-1.583392
H	-2.685378	1.123254	-2.868896

2yH

E = -3334.488975 au

Ni	0.007643	0.003885	-0.008353
S	0.008541	0.000750	2.103521
S	2.173206	-0.178847	-0.057859
S	-1.881665	-0.938905	-0.049423
S	-0.422936	1.055694	-1.861406
C	1.561082	-0.706082	2.581013
C	2.502009	-0.635532	1.600626
C	-2.884058	0.043504	-1.130199
C	-2.152748	0.810598	-1.983564
C	-1.371442	-1.173323	2.597740
C	-2.547846	-0.789776	1.700153
H	-1.040006	-2.202079	2.419503
H	-1.595753	-1.020660	3.657956
H	-2.869846	0.243706	1.868044
H	-3.391809	-1.477549	1.811393
H	1.758352	-0.891737	3.633110
H	3.545620	-0.850683	1.831724
H	-3.936824	-0.199369	-1.244171
H	-2.640057	1.304409	-2.824695

2H

E = -3334.485334 au

Ni	-0.016333	0.043822	0.023745
S	0.009148	-0.044071	2.223776
S	2.159482	0.142190	-0.053907
S	-2.171839	-0.141396	0.166965
S	-0.052715	-0.565018	-2.063796
C	1.687174	-0.460457	2.593718
C	2.575470	-0.295540	1.578908
C	-2.636014	-1.077157	-1.267684
C	-1.697288	-1.124398	-2.243665
C	-0.945395	-1.644140	2.177249
C	-2.337550	-1.307103	1.625904
H	-0.415271	-2.347318	1.527718
H	-1.010167	-2.053627	3.193084
H	-2.948239	-0.780683	2.366402
H	-2.865359	-2.203212	1.284576
H	1.951396	-0.621652	3.634666
H	3.642902	-0.415471	1.771281
H	-3.686472	-1.325775	-1.390830
H	-1.948367	-1.526292	-3.226125

TS_{3H}

E = -3334.462506 au

Ni	-0.009666	0.026659	-0.010262
S	-0.003393	-0.054462	2.142800
S	2.139168	-0.054462	0.124753
S	-2.140722	0.023126	-0.028902
S	0.099165	0.023126	-2.138619
C	1.466683	0.856020	2.538873
C	2.446621	0.856020	1.615882
C	-2.555210	0.071608	-1.722821
C	-1.566936	0.071608	-2.653661
C	1.155629	-1.947856	2.279602
C	2.206416	-1.947856	1.289882
H	1.444799	-1.880418	3.326733
H	0.305760	-2.602839	2.094941
H	2.072908	-2.602839	0.430490
H	3.234381	-1.880418	1.641152
H	1.552749	1.281236	3.536311
H	3.437128	1.281236	1.761442
H	-3.614290	0.104850	-1.970921
H	-1.751259	0.104850	-3.725683

3H

E = -3334.470943 au

Ni	0.001044	-0.012582	0.001178
S	-0.030853	-0.011195	2.189815
S	2.170058	-0.011040	0.295102
S	-2.118988	-0.087865	-0.111248
S	0.205119	-0.087660	-2.112007
C	1.266265	1.216287	2.496962
C	2.280799	1.216375	1.623555
C	-2.467958	-0.154767	-1.832633
C	-1.445230	-0.154680	-2.713070
C	1.119551	-1.489553	2.476255
C	2.282496	-1.489382	1.475320
H	1.457357	-1.441304	3.515839
H	0.465671	-2.356183	2.342443
H	2.247834	-2.356052	0.808842
H	3.260175	-1.440766	1.964148
H	1.183825	1.848968	3.377102

H	3.163353	1.849138	1.672943
H	-3.517389	-0.191375	-2.117562
H	-1.570938	-0.191214	-3.793206

4H

E = -3334.505384 au

Ni	-0.012531	-0.031967	-0.001180
S	-0.016455	-0.014273	2.239537
S	2.207577	-0.004374	0.007094
S	-1.617435	1.501589	0.045641
S	0.056260	0.114991	-2.236088
C	1.643555	-0.313468	2.629869
C	2.599393	-0.363337	1.655061
C	-2.109065	1.607328	-1.611252
C	-1.352496	1.051809	-2.603908
C	-1.359183	-1.521786	-0.038215
C	-0.043648	-2.038453	-0.087511
H	-1.917188	-1.559158	0.895540
H	-1.951611	-1.459676	-0.948880
H	0.361496	-2.388988	-1.034954
H	0.410116	-2.452441	0.810738
H	1.872664	-0.486560	3.681075
H	3.634415	-0.622945	1.872768
H	-3.037828	2.136595	-1.819433
H	-1.612778	1.145827	-3.657901

5H

E = -3334.499911 au

Ni	-0.042746	-0.034294	0.012864
S	0.002609	0.001873	2.301351
S	2.188571	0.095817	-0.071981
S	-2.069557	0.755270	0.008705
S	-0.083379	-0.317554	-2.117515
C	1.724892	-0.247193	2.622065
C	2.605058	-0.172336	1.591917
C	-2.618911	0.449466	-1.618844
C	-1.740548	0.006175	-2.553001
C	-0.661004	-1.719392	1.878157
C	-0.213173	-1.920210	0.454324
H	-0.283295	-2.429566	2.622989
H	-1.746287	-1.604792	1.967941
H	-0.959743	-2.402787	-0.178525
H	0.762313	-2.403462	0.364090
H	2.012913	-0.372712	3.662655
H	3.672944	-0.270306	1.795096
H	-3.672013	0.625445	-1.828835
H	-2.016002	-0.196890	-3.586802

TPSS/6-31++G**

1H

E = -3255.98083850 au

Ni	0.000000	-0.000106	0.000000
S	-0.001340	-0.000195	2.158511
S	2.156858	-0.000115	-0.084449
S	-2.156859	-0.000685	0.084449
S	0.001340	-0.000587	-2.158511
C	1.665786	-0.000233	2.561004
C	2.623244	-0.000198	1.565943
C	-2.623243	-0.001194	-1.565943
C	-1.665786	-0.001150	-2.561004
H	1.931663	-0.000288	3.618005
H	3.689698	-0.000225	1.790925
H	-3.689697	-0.001552	-1.790925
H	-1.931662	-0.001470	-3.618005

TS_{2yH}

E = -3334.55127291 au

Ni	0.012379	0.008714	-0.013534
S	-0.015986	0.036049	2.100902
S	2.180056	-0.060177	-0.067550
S	-1.684281	-1.232895	-0.241887
S	-0.536358	1.217204	-1.729614
C	1.613665	-0.366676	2.586291
C	2.566579	-0.335469	1.602739
C	-2.707857	-0.403544	-1.389938
C	-2.136949	0.637893	-2.072482
C	-1.626641	-1.426253	2.832391
C	-2.630182	-1.570195	1.821875
H	-1.018006	-2.295518	3.075863
H	-1.847615	-0.769270	3.669483
H	-3.439088	-0.841904	1.797371
H	-2.909969	-2.579672	1.532298
H	1.834722	-0.490151	3.644470
H	3.624095	-0.440442	1.849089
H	-3.689119	-0.815190	-1.616935
H	-2.663593	1.116555	-2.899269

2yH

E = -3334.57427532 au

Ni	-0.007435	-0.003666	0.008182
S	0.008648	-0.006829	2.153222
S	2.172280	-0.144851	-0.052906
S	-1.929208	-0.955086	-0.047105
S	-0.413310	1.026056	-1.875899
C	1.580396	-0.705474	2.588987
C	2.512174	-0.607991	1.598723
C	-2.894508	0.047337	-1.147893
C	-2.141678	0.793693	-2.004946
C	-1.375697	-1.197628	2.594496
C	-2.554084	-0.770728	1.714905
H	-1.049104	-2.221573	2.382141
H	-1.608673	-1.086333	3.659012
H	-2.842728	0.272226	1.885645
H	-3.417182	-1.431058	1.852327
H	1.796486	-0.912721	3.634091
H	3.560138	-0.812605	1.825620
H	-3.953316	-0.167543	-1.268883
H	-2.621733	1.282780	-2.854604

2H

E = -3334.57485197 au

Ni	-0.007350	-0.031662	0.016365
S	-0.001974	-0.003958	2.243452
S	2.178208	-0.025600	-0.067695
S	-2.209085	-0.134662	0.179823
S	-0.065656	-0.610395	-2.090479
C	1.687151	-0.381452	2.625177
C	2.578479	-0.318353	1.599440
C	-2.677520	-1.013967	-1.293317
C	-1.732515	-1.090496	-2.265350
C	-0.919824	-1.640916	2.196337
C	-2.311995	-1.354865	1.612937
H	-0.344171	-2.323305	1.563993
H	-0.991149	-2.036052	3.218384
H	-2.970446	-0.889495	2.353802
H	-2.779838	-2.269934	1.234687
H	1.957662	-0.473263	3.673820
H	3.643295	-0.445709	1.807784
H	-3.733279	-1.231495	-1.435299
H	-2.005432	-1.471719	-3.251878

TS_{3H}

E = -3334.54992136 au

Ni	0.001721	0.022254	0.001827
S	0.000521	-0.023411	2.181762

S	2.177827	-0.023411	0.130989
S	-2.145919	0.003436	-0.017646
S	0.110711	0.003436	-2.143134
C	1.476883	0.879200	2.552500
C	2.459614	0.879200	1.626880
C	-2.548654	0.051932	-1.713353
C	-1.557878	0.051932	-2.646551
C	1.139190	-1.959648	2.260481
C	2.188312	-1.959648	1.272328
H	1.430714	-1.917126	3.308439
H	0.265368	-2.576267	2.058394
H	2.038841	-2.576267	0.387985
H	3.216961	-1.917126	1.625999
H	1.576724	1.310946	3.547018
H	3.446382	1.310946	1.786014
H	-3.607000	0.084406	-1.969612
H	-1.750389	0.084406	-3.718328

3H

E = -3334.560871 au

Ni	0.007129	-0.011676	0.008257
S	-0.024756	-0.002764	2.238020
S	2.216806	-0.002650	0.308266
S	-2.126830	-0.091136	-0.109361
S	0.208120	-0.090987	-2.119473
C	1.271568	1.230301	2.505064
C	2.288053	1.230389	1.629936
C	-2.469976	-0.162612	-1.833651
C	-1.445975	-0.162552	-2.715193
C	1.112460	-1.496291	2.470155
C	2.277589	-1.496057	1.467501
H	1.460184	-1.478332	3.508184
H	0.445727	-2.350464	2.319370
H	2.228341	-2.350383	0.785897
H	3.252181	-1.477474	1.966055
H	1.191195	1.885328	3.369999
H	3.155266	1.885492	1.679065
H	-3.519294	-0.201542	-2.122514
H	-1.575598	-0.201439	-3.795799

4H

E = -3334.57556032 au

Ni	-0.002645	-0.006813	-0.000281
S	-0.009538	0.001868	2.243565
S	2.224698	-0.008185	0.007226
S	-1.632685	1.510417	0.045668
S	0.062286	0.131695	-2.238930
C	1.647411	-0.310175	2.631709
C	2.607266	-0.365946	1.656427
C	-2.116572	1.610885	-1.612633
C	-1.352982	1.056985	-2.605474
C	-1.371344	-1.563637	-0.041521
C	-0.063342	-2.077446	-0.087000
H	-1.924744	-1.549307	0.895553
H	-1.952127	-1.452793	-0.954773
H	0.373747	-2.386949	-1.034484
H	0.415073	-2.448076	0.817089
H	1.878170	-0.488492	3.682634
H	3.639554	-0.634141	1.881276
H	-3.048997	2.132478	-1.828572
H	-1.617975	1.148344	-3.659476

5H

E = -3334.57445948 au

Ni	0.000744	-0.007744	0.010496
S	0.000273	0.006931	2.277579
S	2.240342	0.000273	-0.041704
S	-2.047211	0.761781	0.006107
S	-0.026302	-0.281507	-2.132413
C	1.718507	-0.175283	2.655633
C	2.624044	-0.156944	1.641591
C	-2.583828	0.420980	-1.617973
C	-1.695019	-0.005781	-2.554286
C	-0.610260	-1.765381	1.880780
C	-0.373433	-1.927999	0.404640
H	-0.049846	-2.442951	2.533518
H	-1.671984	-1.743339	2.145705
H	-1.246817	-2.214765	-0.181666
H	0.533164	-2.467308	0.127909
H	1.983898	-0.241841	3.708459
H	3.688075	-0.239412	1.874290
H	-3.644417	0.551926	-1.828905
H	-1.977290	-0.229083	-3.583108

TPSS/cc-pVDZ

1H

E = -3256.275118 au

Ni	0.000000	-0.000294	0.000000
S	0.003117	-0.000141	2.169331
S	2.167741	-0.000132	-0.083103
S	-2.167741	-0.000722	0.083103
S	-0.003117	-0.000713	-2.169331
C	1.674780	0.000033	2.567352
C	2.631886	0.000037	1.571420
C	-2.631886	-0.001119	-1.571420
C	-1.674780	-0.001115	-2.567352
H	1.941022	0.000142	3.631287
H	3.705562	0.000149	1.795167
H	-3.705562	-0.001369	-1.795167
H	-1.941022	-0.001362	-3.631287

TS_{2yH}

E = -3334.840922 au

Ni	0.017107	0.012042	-0.018704
S	-0.015589	0.034672	2.111243
S	2.198656	-0.041354	-0.059686
S	-1.693506	-1.237733	-0.242575
S	-0.537677	1.210545	-1.756373
C	1.617531	-0.369270	2.595158
C	2.573884	-0.327798	1.614232
C	-2.717412	-0.404955	-1.392585
C	-2.144151	0.630294	-2.084088
C	-1.620853	-1.440769	2.828777
C	-2.636326	-1.555930	1.825877
H	-1.009486	-2.323333	3.050428
H	-1.825244	-0.790793	3.684866
H	-3.435159	-0.805326	1.809195
H	-2.939474	-2.563171	1.524715
H	1.837032	-0.496677	3.660183
H	3.637808	-0.429349	1.866417
H	-3.705896	-0.818847	-1.616831
H	-2.675392	1.106809	-2.918689

2yH

E = -3334.863248 au

Ni	-0.000160	-0.000022	0.000204
S	0.012208	-0.005247	2.163385
S	2.194348	-0.120870	-0.044044
S	-1.938305	-0.959442	-0.051197
S	-0.415519	1.012025	-1.906537
C	1.584870	-0.716571	2.593174
C	2.520644	-0.605541	1.607017
C	-2.903608	0.056115	-1.147006
C	-2.149658	0.791490	-2.013776
C	-1.377762	-1.199700	2.594428
C	-2.554488	-0.769893	1.717679
H	-1.044982	-2.228077	2.375224

H	-1.608219	-1.091912	3.667151
H	-2.839961	0.282180	1.885007
H	-3.426819	-1.430080	1.854259
H	1.799388	-0.929487	3.644587
H	3.575188	-0.809574	1.839424
H	-3.970080	-0.157723	-1.264178
H	-2.635618	1.280334	-2.869685

2H

E = -3334.864760 au

Ni	-0.003378	-0.015927	0.009713
S	0.001291	0.003782	2.251764
S	2.192870	-0.006213	-0.068031
S	-2.220556	-0.133608	0.175934
S	-0.069279	-0.581875	-2.111984
C	1.692201	-0.395797	2.625919
C	2.584309	-0.320801	1.600893
C	-2.674716	-1.033342	-1.294601
C	-1.732725	-1.090649	-2.272079
C	-0.926078	-1.633493	2.200302
C	-2.317188	-1.349538	1.618671
H	-0.342952	-2.317659	1.563999
H	-0.994741	-2.031248	3.228985
H	-2.980097	-0.873186	2.359271
H	-2.792493	-2.269007	1.240111
H	1.963742	-0.502155	3.680057
H	3.655762	-0.451778	1.811032
H	-3.734245	-1.268508	-1.433501
H	-2.007163	-1.476296	-3.264472

TS_{3H}

E = -3334.840448 au

Ni	-0.005591	0.011904	-0.005936
S	-0.000199	-0.037987	2.187309
S	2.183407	-0.037987	0.130603
S	-2.162751	0.002765	-0.027515
S	0.101867	0.002765	-2.160526
C	1.477210	0.873859	2.553328
C	2.460421	0.873859	1.627255
C	-2.561798	0.062307	-1.726941
C	-1.570655	0.062307	-2.660484
C	1.151088	-1.960328	2.273979
C	2.201074	-1.960328	1.285012
H	1.442066	-1.908117	3.329073
H	0.273725	-2.585562	2.074046
H	2.053965	-2.585562	0.397263
H	3.236879	-1.908117	1.638564
H	1.576806	1.310838	3.553385
H	3.452733	1.310838	1.786477
H	-3.626882	0.100867	-1.983873
H	-1.763435	0.100867	-3.739027

3H

E = -3334.850557 au

Ni	0.001277	-0.011764	0.001463
S	-0.024274	-0.004372	2.247258
S	2.225875	-0.004234	0.310133
S	-2.141418	-0.091174	-0.118737
S	0.201035	-0.091001	-2.135289
C	1.276380	1.230165	2.511512
C	2.293699	1.230253	1.635687
C	-2.481422	-0.161702	-1.846775
C	-1.457228	-0.161631	-2.728475
C	1.120511	-1.498284	2.477718
C	2.283828	-1.498083	1.476534
H	1.465432	-1.475693	3.523731
H	0.444519	-2.354155	2.326773
H	2.235650	-2.354056	0.785697
H	3.266777	-1.475000	1.973422
H	1.198514	1.888467	3.383240
H	3.167254	1.888635	1.688323
H	-3.537672	-0.200675	-2.136383
H	-1.586548	-0.200547	-3.816050

4H

E = -3334.863705 au

Ni	-0.006487	-0.016564	-0.000625
S	-0.007287	-0.002150	2.254855
S	2.235078	-0.008243	0.008711
S	-1.640285	1.517537	0.044431
S	0.058174	0.130987	-2.250387
C	1.656094	-0.300457	2.639552
C	2.616639	-0.355505	1.663208
C	-2.116150	1.625301	-1.618539
C	-1.352520	1.070469	-2.612498
C	-1.378739	-1.584866	-0.039056
C	-0.072341	-2.097818	-0.090931
H	-1.929583	-1.568789	0.907566
H	-1.966555	-1.468870	-0.955410
H	0.364297	-2.403725	-1.047775
H	0.414656	-2.469670	0.816398
H	1.889514	-0.474132	3.697959
H	3.657262	-0.617542	1.891302
H	-3.050396	2.157262	-1.837141
H	-1.616115	1.167485	-3.673620

5H

E = -3334.863249 au

Ni	-0.003145	-0.009999	0.004436
S	0.000802	0.009199	2.284941
S	2.249786	0.009670	-0.047678
S	-2.065238	0.758095	-0.000158
S	-0.032261	-0.270636	-2.149521
C	1.723964	-0.183248	2.654649
C	2.628611	-0.158274	1.638873
C	-2.595704	0.426642	-1.631076
C	-1.704068	0.008249	-2.569651
C	-0.614180	-1.768191	1.890987
C	-0.360461	-1.934579	0.419132
H	-0.059851	-2.443258	2.563221
H	-1.684024	-1.731586	2.151370
H	-1.228651	-2.246410	-0.175471
H	0.562696	-2.468203	0.158476
H	1.992552	-0.260909	3.713034
H	3.699681	-0.243237	1.872267
H	-3.662871	0.559115	-1.843938
H	-1.984996	-0.209888	-3.607241

TPSS/aug-cc-pVDZ

1H

E = -3256.292577 au

Ni	0.000000	-0.000280	0.000000
S	0.001511	-0.000155	2.164633
S	2.162983	-0.000146	-0.084521
S	-2.162983	-0.000734	0.084521
S	-0.001511	-0.000725	-2.164633
C	1.673505	0.000033	2.565991
C	2.630475	0.000037	1.570200
C	-2.630475	-0.001118	-1.570200
C	-1.673505	-0.001114	-2.565991
H	1.936659	0.000149	3.628616
H	3.702720	0.000157	1.790913
H	-3.702719	-0.001359	-1.790913
H	-1.936659	-0.001352	-3.628616

TS_{2yH}

E = -3334.864359 au

Ni	0.017171	0.012087	-0.018775
S	-0.016460	0.027103	2.104958
S	2.195961	-0.034982	-0.057641
S	-1.692137	-1.229812	-0.236838
S	-0.535312	1.203939	-1.758056
C	1.619093	-0.363914	2.595299
C	2.576615	-0.318840	1.616893
C	-2.715126	-0.407601	-1.396933
C	-2.142327	0.624542	-2.091728
C	-1.625138	-1.457803	2.833094
C	-2.647645	-1.549880	1.838622
H	-1.016487	-2.342781	3.033558
H	-1.805160	-0.809973	3.691922
H	-3.429826	-0.787052	1.827890
H	-2.960399	-2.544583	1.518578
H	1.833627	-0.492420	3.659002
H	3.639415	-0.417636	1.864574
H	-3.701834	-0.822641	-1.616367
H	-2.668179	1.101305	-2.926490

2yH

E = -3334.887922 au

Ni	0.002481	0.001301	-0.002692
S	0.010240	-0.009727	2.150953
S	2.195919	-0.118204	-0.040155
S	-1.928658	-0.951115	-0.047187
S	-0.418196	1.008805	-1.909213
C	1.582915	-0.717247	2.592633
C	2.522955	-0.603823	1.611977
C	-2.903039	0.056097	-1.144946
C	-2.153818	0.788846	-2.016710
C	-1.377330	-1.201942	2.593344
C	-2.554514	-0.767448	1.718318
H	-1.051316	-2.228224	2.373892
H	-1.602976	-1.089000	3.663000
H	-2.837660	0.280308	1.890762
H	-3.422888	-1.428396	1.848350
H	1.788095	-0.935812	3.642311
H	3.575441	-0.806385	1.843095
H	-3.968542	-0.156285	-1.251206
H	-2.637644	1.276257	-2.871412

2H

E = -3334.889046 au

Ni	-0.001297	-0.024089	0.007059
S	-0.002190	0.010843	2.238066
S	2.193563	-0.036405	-0.067930
S	-2.206781	-0.130129	0.181444
S	-0.074153	-0.598358	-2.109869
C	1.688678	-0.382819	2.628818
C	2.584692	-0.325084	1.607295
C	-2.682144	-1.017342	-1.292283
C	-1.744856	-1.086108	-2.272534
C	-0.919499	-1.630609	2.203203
C	-2.309489	-1.361764	1.609666
H	-0.333953	-2.317806	1.579397
H	-0.992889	-2.013567	3.233688
H	-2.985891	-0.908766	2.347219
H	-2.759150	-2.282336	1.212994
H	1.951343	-0.477554	3.683853
H	3.653327	-0.456843	1.818467
H	-3.742719	-1.240717	-1.423586
H	-2.022027	-1.467846	-3.262985

TS_{3H}

E = -3334.864857 au

Ni	-0.001027	0.027463	-0.001091
S	0.001448	-0.017709	2.184068
S	2.180073	-0.017709	0.132053
S	-2.156176	0.007133	-0.021095
S	0.107882	0.007133	-2.153579
C	1.485180	0.875936	2.561861
C	2.468462	0.875936	1.635721
C	-2.557086	0.048021	-1.721790
C	-1.565795	0.048021	-2.655473
C	1.141931	-1.959475	2.262431
C	2.190095	-1.959475	1.275181
H	1.430467	-1.907583	3.314471
H	0.259810	-2.570012	2.057998
H	2.038779	-2.570012	0.382414
H	3.222998	-1.907583	1.626112
H	1.586860	1.297963	3.565262
H	3.463987	1.297963	1.797223
H	-3.620682	0.076590	-1.977331
H	-1.757276	0.076590	-3.732447

3H

E = -3334.875797 au

Ni	0.004390	-0.007996	0.005083
S	-0.025489	0.002810	2.239626
S	2.218507	0.002946	0.307795
S	-2.137915	-0.090380	-0.112411
S	0.206767	-0.090212	-2.130881
C	1.278435	1.232630	2.513302
C	2.295166	1.232720	1.637978
C	-2.477201	-0.167300	-1.841459
C	-1.452600	-0.167231	-2.723509
C	1.114500	-1.495494	2.470760
C	2.277846	-1.495289	1.469560
H	1.460814	-1.473197	3.512804
H	0.441161	-2.348839	2.318277
H	2.227766	-2.348741	0.781121
H	3.256657	-1.472491	1.967246
H	1.202851	1.879741	3.390296
H	3.173590	1.879911	1.693653
H	-3.531366	-0.209281	-2.130521
H	-1.581690	-0.209156	-3.808941

4H

E = -3334.888036 au

Ni	0.000574	0.001285	-0.000007
S	0.000843	0.020719	2.251317
S	2.237830	-0.027881	0.010737
S	-1.655476	1.505299	0.041301
S	0.067734	0.153020	-2.245295
C	1.658176	-0.311123	2.640918
C	2.617880	-0.380403	1.666519
C	-2.133941	1.608181	-1.623277
C	-1.361335	1.064151	-2.614436
C	-1.370581	-1.562257	-0.042158
C	-0.062985	-2.075979	-0.086329
H	-1.926687	-1.546938	0.897259
H	-1.952445	-1.449256	-0.958526
H	0.376815	-2.386440	-1.036161
H	0.417592	-2.446007	0.820970
H	1.884125	-0.487827	3.698025
H	3.653229	-0.657108	1.889967
H	-3.074458	2.125548	-1.838214
H	-1.621634	1.153730	-3.674611

5H

E = -3334.887807 au

Ni	-0.000021	-0.007485	0.005067
S	0.001364	0.017163	2.277467
S	2.248508	-0.008692	-0.045042
S	-2.065758	0.740012	0.005579

S	-0.025623	-0.252999	-2.149694
C	1.723990	-0.180865	2.656382
C	2.630438	-0.166822	1.643355
C	-2.596984	0.412747	-1.628382
C	-1.702670	0.007260	-2.568704
C	-0.612606	-1.761621	1.889988
C	-0.365926	-1.927996	0.416786
H	-0.051024	-2.433539	2.553268
H	-1.678433	-1.732037	2.151761
H	-1.235510	-2.225938	-0.175828
H	0.550741	-2.461574	0.149478
H	1.985381	-0.253685	3.714378
H	3.699350	-0.255155	1.873690
H	-3.663399	0.540079	-1.836760
H	-1.979174	-0.206300	-3.606137

TPSS/cc-pVTZ

1H

E = -3256.390522 au

Ni	0.000000	-0.000101	0.000000
S	0.004539	-0.000148	2.149931
S	2.148413	-0.000139	-0.080911
S	-2.148413	-0.000724	0.080911
S	-0.004539	-0.000715	-2.149931
C	1.663828	0.000012	2.551495
C	2.615606	0.000016	1.561107
C	-2.615606	-0.001133	-1.561107
C	-1.663828	-0.001129	-2.551495
H	1.925589	0.000110	3.606585
H	3.680266	0.000118	1.780727
H	-3.680266	-0.001390	-1.780727
H	-1.925589	-0.001383	-3.606585

TS_{2yH}

E = -3334.981882 au

Ni	0.016462	0.011588	-0.017999
S	-0.007509	0.018836	2.091893
S	2.183661	-0.046054	-0.050196
S	-1.688142	-1.212433	-0.237925
S	-0.543997	1.200241	-1.742556
C	1.613559	-0.371387	2.584094
C	2.565331	-0.330576	1.611169
C	-2.708509	-0.399366	-1.386912
C	-2.140919	0.629327	-2.075207
C	-1.630850	-1.435015	2.830428
C	-2.632090	-1.565739	1.830526
H	-1.023114	-2.302330	3.068104
H	-1.828158	-0.769744	3.662394
H	-3.435035	-0.835835	1.806284
H	-2.909452	-2.565139	1.517547
H	1.825920	-0.500145	3.640339
H	3.620737	-0.429807	1.856650
H	-3.688731	-0.811119	-1.603605
H	-2.663312	1.103754	-2.903466

2yH

E = -3335.006695 au

Ni	0.000482	0.000299	-0.000500
S	0.010201	-0.033277	2.134822
S	2.183032	-0.116259	-0.027959
S	-1.923847	-0.925176	-0.036288
S	-0.425923	0.996534	-1.898804
C	1.574024	-0.717190	2.585546
C	2.509955	-0.596416	1.613379
C	-2.895037	0.055595	-1.136883
C	-2.149644	0.777018	-2.008433
C	-1.373729	-1.207486	2.582305
C	-2.547575	-0.756625	1.717799
H	-1.063721	-2.229992	2.355940
H	-1.588513	-1.102480	3.648063
H	-2.820042	0.284687	1.902996
H	-3.417713	-1.405079	1.841752
H	1.774952	-0.939093	3.627392
H	3.556860	-0.784004	1.846573
H	-3.954116	-0.152361	-1.237693
H	-2.628180	1.249311	-2.864892

2H

E = -3335.007004 au

Ni	-0.002700	-0.028977	0.007576
S	0.002973	-0.014705	2.218134
S	2.179964	-0.030723	-0.065881
S	-2.187779	-0.155527	0.176606
S	-0.078789	-0.574761	-2.104130
C	1.681903	-0.394842	2.610972
C	2.572705	-0.321757	1.596742
C	-2.662242	-1.029038	-1.289041
C	-1.733879	-1.075829	-2.267540
C	-0.925686	-1.634690	2.211677
C	-2.307555	-1.357179	1.613123
H	-0.353123	-2.337652	1.606092
H	-1.003162	-1.999381	3.241314
H	-2.973380	-0.885725	2.338460
H	-2.771574	-2.271107	1.237090
H	1.944229	-0.492215	3.658052
H	3.635595	-0.439177	1.806822
H	-3.713097	-1.262634	-1.417943
H	-2.009842	-1.441379	-3.256144

TS_{3H}

E = -3334.980922 au

Ni	-0.005342	0.011589	-0.005672
S	0.001269	-0.030672	2.164905
S	2.160955	-0.030672	0.130729
S	-2.146803	0.004006	-0.031079
S	0.097355	0.004006	-2.144820
C	1.470951	0.863283	2.540349
C	2.447839	0.863283	1.620231
C	-2.548144	0.061515	-1.718360
C	-1.562906	0.061515	-2.646342
C	1.154757	-1.956195	2.269763
C	2.196646	-1.956195	1.288422
H	1.437283	-1.889846	3.315224
H	0.284419	-2.574627	2.076264
H	2.055540	-2.574627	0.408071
H	3.223341	-1.889846	1.632961
H	1.572785	1.282258	3.537074
H	3.436691	1.282258	1.781487
H	-3.604125	0.099078	-1.971635
H	-1.752580	0.099078	-3.715579

3H

E = -3334.992658 au

Ni	0.004782	-0.011335	0.005538
S	-0.018015	-0.001443	2.227133
S	2.205033	-0.001317	0.313319
S	-2.123226	-0.091434	-0.120443
S	0.196635	-0.091278	-2.117550
C	1.276358	1.220606	2.503831
C	2.286112	1.220691	1.634509
C	-2.466930	-0.164873	-1.836419
C	-1.449151	-0.164808	-2.712599
C	1.113829	-1.486608	2.467000
C	2.274243	-1.486391	1.468355
H	1.456873	-1.462967	3.502867
H	0.448772	-2.338808	2.319874

H	2.228288	-2.338720	0.788929
H	3.247416	-1.462188	1.961913
H	1.201981	1.863451	3.374965
H	3.158566	1.863614	1.690495
H	-3.514268	-0.205577	-2.121282
H	-1.575108	-0.205464	-3.790655

4H

E = -3334.998907 au

Ni	0.001810	0.004414	0.000102
S	0.007847	0.022233	2.239864
S	2.227327	-0.034491	0.016004
S	-1.652159	1.493651	0.035391
S	0.063367	0.158199	-2.233609
C	1.653560	-0.305461	2.630024
C	2.607396	-0.376454	1.661682
C	-2.123697	1.603619	-1.618457
C	-1.354367	1.064466	-2.603328
C	-1.367240	-1.565752	-0.040631
C	-0.067774	-2.076160	-0.087989
H	-1.917304	-1.548498	0.894409
H	-1.947570	-1.452007	-0.949613
H	0.368819	-2.381359	-1.033192
H	0.412364	-2.444153	0.812021
H	1.877983	-0.480779	3.679838
H	3.635267	-0.651437	1.884523
H	-3.057587	2.117111	-1.832861
H	-1.612787	1.153569	-3.656178

5H

E = -3335.000365 au

Ni	-0.001354	-0.008859	0.005584
S	0.006667	0.002588	2.265993
S	2.236869	-0.008964	-0.041674
S	-2.056940	0.731426	-0.001801
S	-0.031481	-0.249942	-2.136863
C	1.717495	-0.181555	2.642753
C	2.617924	-0.161589	1.635031
C	-2.584144	0.414945	-1.625806
C	-1.694056	0.012896	-2.559693
C	-0.609902	-1.762445	1.891079
C	-0.369046	-1.933339	0.422860
H	-0.058150	-2.434155	2.551714
H	-1.668510	-1.730193	2.153783
H	-1.233814	-2.232612	-0.162904
H	0.540253	-2.464585	0.154164
H	1.980590	-0.252555	3.692710
H	3.680172	-0.241639	1.864267
H	-3.642867	0.541151	-1.834001
H	-1.967064	-0.198023	-3.590545

TPSS/aug-cc-pVTZ

1H

E = -3256.395424 au

Ni	0.000000	-0.000091	0.000000
S	0.004632	-0.000157	2.148840
S	2.147326	-0.000148	-0.080775
S	-2.147326	-0.000733	0.080775
S	-0.004632	-0.000724	-2.148840
C	1.663522	0.000012	2.551287
C	2.615386	0.000017	1.560809
C	-2.615386	-0.001132	-1.560809
C	-1.663522	-0.001129	-2.551287
H	1.925297	0.000116	3.606306
H	3.679976	0.000123	1.780447
H	-3.679976	-0.001384	-1.780447
H	-1.925296	-0.001377	-3.606306

TS_{2yH}

E = -3334.987373 au

Ni	0.000000	0.510648	0.000000
S	1.358264	-0.907224	0.768848
18			18
S	1.618726	1.832525	-0.576722
S	-1.358264	-0.907225	-0.768849
S	-1.618726	1.832525	0.576722
C	2.927884	-0.410993	0.210435
C	3.009327	0.837143	-0.327575
C	-2.927885	-0.410994	-0.210435
C	-3.009328	0.837143	0.327574
C	0.701417	-3.015633	0.111766
C	-0.701416	-3.015633	-0.111767
H	1.359792	-3.171361	-0.737016
H	1.066205	-3.403569	1.055135
H	-1.359792	-3.171361	0.737016
H	-1.066205	-3.403569	-1.055136
H	3.785686	-1.040594	0.422766
H	3.972502	1.276228	-0.579128
H	-3.785686	-1.040594	-0.422766
H	-3.972502	1.276228	0.579128

2yH

E = -3335.012580 au

Ni	-0.000111	0.000002	0.000150
S	0.009717	-0.036461	2.133774
S	2.182822	-0.110509	-0.026103
S	-1.924120	-0.922371	-0.034410
S	-0.425195	0.991045	-1.901227
C	1.574042	-0.718408	2.585131
C	2.510635	-0.593516	1.614208
C	-2.895167	0.056756	-1.136346
C	-2.149326	0.774618	-2.010356
C	-1.374122	-1.209675	2.581581
C	-2.547749	-0.754719	1.719145
H	-1.066145	-2.232249	2.352620
H	-1.587158	-1.105999	3.647743
H	-2.817547	0.286979	1.906239
H	-3.419114	-1.401584	1.842123
H	1.774640	-0.943228	3.626435
H	3.557680	-0.779445	1.847642
H	-3.954891	-0.148771	-1.235545
H	-2.627425	1.245540	-2.867687

2H

E = -3335.012853 au

Ni	-0.002629	-0.030518	0.007600
S	0.003229	-0.016776	2.216426
S	2.179487	-0.027858	-0.065657
S	-2.185850	-0.156760	0.176197
S	-0.078863	-0.574269	-2.103935
C	1.682186	-0.396146	2.610168
C	2.573269	-0.320469	1.596424
C	-2.661660	-1.029489	-1.289506
C	-1.733857	-1.075283	-2.268551
C	-0.926421	-1.635659	2.212502
C	-2.307684	-1.356786	1.613519
H	-0.354643	-2.340635	1.608468
H	-1.004509	-1.997972	3.242894
H	-2.972707	-0.883504	2.338359
H	-2.773183	-2.270438	1.238615
H	1.944623	-0.494331	3.657203
H	3.636158	-0.436593	1.806666
H	-3.712419	-1.263811	-1.418094
H	-2.009962	-1.440003	-3.257314

TS_{3H}

E = -3334.987016 au

Ni	-0.004929	0.010226	-0.005233
S	0.000980	-0.029773	2.163916
S	2.159985	-0.029773	0.130380
S	-2.145628	0.004012	-0.030298
S	0.098064	0.004012	-2.143600
C	1.470059	0.863714	2.539527
C	2.447073	0.863714	1.619292
C	-2.547399	0.061519	-1.717355
C	-1.561947	0.061519	-2.645539
C	1.154850	-1.957553	2.269607
C	2.196485	-1.957553	1.288506
H	1.436650	-1.889286	3.315071
H	0.283549	-2.574582	2.076128
H	2.055456	-2.574582	0.407194
H	3.223226	-1.889286	1.632320
H	1.572722	1.282301	3.536400
H	3.436023	1.282301	1.781385
H	-3.603224	0.099130	-1.971066
H	-1.752066	0.099130	-3.714645

3H

E = -3334.998975 au

Ni	0.005470	-0.012408	0.006339
S	-0.018411	-0.002844	2.226368
S	2.204334	-0.002720	0.312812
S	-2.121978	-0.091791	-0.118947
S	0.197927	-0.091638	-2.116091
C	1.274604	1.220486	2.501803
C	2.284368	1.220571	1.632469
C	-2.465820	-0.163806	-1.834762
C	-1.447678	-0.163743	-2.711253
C	1.113784	-1.487191	2.466953
C	2.274206	-1.486971	1.468308
H	1.456756	-1.462427	3.502785
H	0.449158	-2.339870	2.320534
H	2.228900	-2.339781	0.789417
H	3.247352	-1.461632	1.961795
H	1.200298	1.864167	3.372432
H	3.156312	1.864329	1.688447
H	-3.512924	-0.203846	-2.120433
H	-1.574467	-0.203734	-3.789196

4H

E = -3335.004317 au

Ni	0.003328	0.008263	0.000237
S	0.009671	0.028372	2.239031
S	2.228104	-0.038387	0.016722
S	-1.655349	1.491393	0.034457
S	0.066194	0.163871	-2.232362
C	1.653450	-0.307267	2.630232
C	2.607259	-0.382080	1.662284
C	-2.127417	1.599461	-1.619400
C	-1.355520	1.063083	-2.603647
C	-1.365510	-1.561289	-0.040400
C	-0.065991	-2.071713	-0.087911
H	-1.915783	-1.544715	0.894624
H	-1.945511	-1.446664	-0.949580
H	0.370292	-2.377549	-1.033144
H	0.414500	-2.438857	0.812357
H	1.877124	-0.483859	3.679941
H	3.633900	-0.661200	1.885439
H	-3.063219	2.109116	-1.834394
H	-1.614269	1.150734	-3.656485

5H

E = -3335.005894 au

Ni	-0.000641	-0.009391	0.004786
S	0.006904	0.002963	2.263908
S	2.237076	-0.012620	-0.041668
S	-2.056738	0.727075	-0.000777
S	-0.030219	-0.245002	-2.137580
C	1.717390	-0.180798	2.642409
C	2.618289	-0.162576	1.635167
C	-2.584275	0.412606	-1.625066
C	-1.693401	0.014310	-2.559907
C	-0.610062	-1.761675	1.891379
C	-0.370021	-1.933251	0.423248
H	-0.057907	-2.433302	2.551704
H	-1.668546	-1.729110	2.154548
H	-1.235266	-2.231209	-0.162671
H	0.539125	-2.464661	0.154017
H	1.980171	-0.250197	3.692585
H	3.680344	-0.242946	1.864767
H	-3.643170	0.537169	-1.833127
H	-1.966410	-0.194834	-3.591071

B3LYP/6-31++G**

1H

E = -3255.867514 au

Ni	.000000	.000000	.000144
S	1.507510	-1.566716	-.000035
S	1.507510	1.566716	-.000165
S	-1.507510	-1.566716	-.000120
S	-1.507510	1.566716	-.000073
C	2.971874	-.688673	-.000552
C	2.971874	.688673	-.000610
C	-2.971874	-.688673	-.000586
C	-2.971874	.688673	-.000562
H	3.900211	-1.255043	-.000839
H	3.900211	1.255043	-.000950
H	-3.900211	-1.255043	-.000913
H	-3.900211	1.255043	-.000863

TS_{2yH}

E = -3334.419568 au

Ni	.000000	.485834	.000000
S	1.395276	-.940669	.773864
S	1.603464	1.870012	-.550361
S	-1.395274	-.940670	-.773864
S	-1.603466	1.870010	.550361
C	2.945197	-.373457	.225122
C	3.002437	.880430	-.308904
C	-2.945196	-.373460	-.225122
C	-3.002438	.880428	.308905
C	.701481	-3.087561	.092465
C	-.701479	-3.087562	-.092466
H	1.340613	-3.238695	-.772349
H	1.094026	-3.457212	1.031873
H	-1.340610	-3.238696	.772349
H	-1.094023	-3.457213	-1.031874
H	3.826578	-.970600	.437404
H	3.963593	1.326365	-.559006
H	-3.826577	-.970604	-.437404
H	-3.963594	1.326361	.559007

2yH

E = -3334.459012 au

Ni	-.000022	-.531289	-.001171
S	1.348172	.995876	-.806229
S	1.687024	-1.939604	.224016
S	-1.348452	1.000173	.795340
S	-1.686883	-1.941083	-.218336
C	2.936604	.494008	-.199041
C	3.025670	-.820637	.116562
C	-2.936781	.494753	.190829

C	-3.025667	-.821668	-.117346
C	.762201	2.535494	.062076
C	-.762566	2.535056	-.081374
H	1.075538	2.505759	1.109081
H	1.200571	3.409356	-.426716
H	-1.075885	2.499581	-1.128207
H	-1.200998	3.411546	.402630
H	3.785253	1.153179	-.343264
H	4.009146	-1.248975	.306281
H	-3.785526	1.154599	.331352
H	-4.009075	-1.251199	-.304701

2H

E = -3334.463648 au

Ni	0.035660	-0.422400	-0.335816
S	1.424490	1.364909	-0.440324
S	1.714967	-1.786112	0.101117
S	-1.620463	1.074060	-0.652804
S	-1.403434	-1.971378	0.293943
C	2.907690	0.700561	0.263821
C	2.984610	-0.641594	0.415611
C	-2.970275	0.302634	0.205924
C	-2.842905	-1.011202	0.492347
C	0.458479	2.118870	0.967429
C	-0.950676	2.432929	0.450404
H	0.439844	1.396271	1.785239
H	0.964163	3.032811	1.295505
H	-0.953872	3.337854	-0.161886
H	-1.650470	2.566272	1.278787
H	3.745635	1.376064	0.394364
H	3.924734	-1.075603	0.756601
H	-3.903214	0.852475	0.265786
H	-3.708467	-1.550462	0.877212

TS_{3H}

E = -3334.423119 au

Ni	0.303552	0.000000	-0.117606
S	-1.297320	-1.514613	-0.269527
S	-1.297320	1.514613	-0.269526
S	1.790975	-1.564652	0.045558
S	1.790975	1.564651	0.045559
C	-2.450435	-0.674923	-1.287096
C	-2.450434	0.674924	-1.287095
C	3.286492	-0.677656	0.104808
C	3.286492	0.677655	0.104808
C	-2.319205	-0.710885	1.651286
C	-2.319204	0.710885	1.651286
H	-3.260506	-1.228224	1.497875
H	-1.613565	-1.221956	2.298058
H	-1.613564	1.221956	2.298058
H	-3.260505	1.228225	1.497876
H	-3.200972	-1.265677	-1.805214
H	-3.200972	1.265678	-1.805214
H	4.204084	-1.259527	0.139268
H	4.204084	1.259526	0.139269

3H

E = -3334.446488 au

Ni	0.340053	-0.000064	-0.076196
S	-1.403736	-1.501033	-0.049222
S	-1.403168	1.501372	-0.048540
S	1.828570	-1.555326	-0.014807
S	1.829038	1.554716	-0.014111
C	-2.423484	-0.667357	-1.274677
C	-2.423147	0.668628	-1.274465
C	3.350870	-0.671872	0.047253
C	3.351074	0.670776	0.047559
C	-2.228159	-0.769131	1.461979
C	-2.228626	0.769128	1.461929
H	-3.241886	-1.172916	1.506960
H	-1.648183	-1.170932	2.295408
H	-1.649912	1.171306	2.296057
H	-3.242633	1.172329	1.505660
H	-3.016463	-1.278105	-1.948339
H	-3.015825	1.279896	-1.947922
H	4.259080	-1.267683	0.080147
H	4.259459	1.266303	0.080744

4H

E = -3334.442178 au

Ni	0.101476	0.143774	-0.147595
S	-1.603372	-1.377189	-0.377715
S	-1.369470	1.858231	-0.242745
S	1.551825	-1.366601	-0.821991
S	1.682932	1.542637	0.336668
C	-3.031316	-0.335800	-0.314246
C	-2.878844	1.006470	-0.270529
C	3.066004	-0.692106	-0.283682
C	3.123245	0.572230	0.190392
C	-1.091815	-1.610980	1.440097
C	-0.135148	-0.491744	1.733580
H	-2.010228	-1.607656	2.031167
H	-0.616950	-2.593973	1.464733
H	0.841682	-0.790614	2.104169
H	-0.553518	0.359127	2.265154
H	-3.996081	-0.830023	-0.363382
H	-3.768408	1.636203	-0.255610
H	3.940866	-1.334750	-0.335655
H	4.048945	1.030699	0.530050

5H

E = -3334.431478 au

Ni	-0.000051	-0.000045	0.080008
S	-1.653685	-1.532559	0.005292
S	-1.411891	1.546913	-0.744269
S	1.411877	-1.546154	-0.745665
S	1.653479	1.532658	0.006700
C	-3.041759	-0.569993	-0.344579
C	-2.942833	0.765085	-0.611442
C	2.942749	-0.764284	-0.612368
C	3.041591	0.570555	-0.344276
C	0.453698	-0.524834	2.096954
C	-0.453708	0.522818	2.097494
H	0.118319	-1.548256	2.229257
H	1.515272	-0.338816	2.216394
H	-0.118321	1.546109	2.230785
H	-1.515280	0.336685	2.216769
H	-4.005826	-1.073621	-0.312069
H	-3.829982	1.378555	-0.751528
H	3.829936	-1.377543	-0.753143
H	4.005619	1.074235	-0.311420

B3PW91/6-31++G**

1H

E = -3255.568343 au

Ni	0.000000	-0.000072	0.000000
S	-0.005534	-0.000164	2.149686
S	2.147879	-0.000082	-0.088300
S	-2.147879	-0.000649	0.088301
S	0.005534	-0.000554	-2.149686
C	1.648821	-0.000244	2.540907
C	2.602508	-0.000209	1.549765
C	-2.602507	-0.001196	-1.549765
C	-1.648821	-0.001153	-2.540906
H	1.921357	-0.000327	3.594180
H	3.665494	-0.000263	1.781544

H	-3.665494	-0.001582	-1.781544
H	-1.921356	-0.001502	-3.594180

TS_{2yH}

E = -3334.092300 au

Ni	-0.006123	-0.004310	0.006695
S	0.004680	-0.002502	2.119221
S	2.153758	-0.034014	-0.086973
S	-1.724643	-1.208208	-0.238672
S	-0.500134	1.198028	-1.721044
C	1.641385	-0.347036	2.554848
C	2.571891	-0.311255	1.558728
C	-2.679148	-0.383463	-1.420193
C	-2.089880	0.650551	-2.085743
C	-1.695077	-1.466842	2.887379
C	-2.678530	-1.611812	1.894574
H	-1.078050	-2.322707	3.145262
H	-1.864408	-0.751665	3.683753
H	-3.494291	-0.895839	1.853979
H	-2.908043	-2.607743	1.534282
H	1.894616	-0.457714	3.605177
H	3.632167	-0.408933	1.786993
H	-3.655597	-0.781870	-1.679780
H	-2.598721	1.136392	-2.916928

2yH

E = -3334.137175 au

Ni	-0.010522	-0.005691	0.011682
S	-0.005477	-0.013385	2.167932
S	2.174642	-0.005478	-0.024940
S	-1.910434	-1.023933	-0.043199
S	-0.431194	0.949442	-1.908485
C	1.583214	-0.650854	2.586130
C	2.507702	-0.499274	1.608310
C	-2.880992	-0.051780	-1.146890
C	-2.147966	0.694067	-2.007222
C	-1.330800	-1.236386	2.572365
C	-2.516156	-0.846475	1.693863
H	-0.975083	-2.247715	2.354457
H	-1.584198	-1.157245	3.633119
H	-2.832396	0.186229	1.867992
H	-3.362169	-1.520879	1.852336
H	1.808360	-0.875909	3.623049
H	3.557260	-0.676399	1.842259
H	-3.935815	-0.275932	-1.263712
H	-2.647212	1.169145	-2.851456

2H

E = -3334.140848 au

Ni	-0.006841	-0.021336	0.011717
S	-0.005981	-0.008344	2.242973
S	2.176067	-0.021175	-0.064350
S	-2.216841	-0.142354	0.184369
S	-0.075478	-0.572054	-2.100009
C	1.672505	-0.391592	2.612113
C	2.559098	-0.327268	1.593322
C	-2.660425	-1.022497	-1.280701
C	-1.723533	-1.084644	-2.250356
C	-0.916817	-1.620132	2.191739
C	-2.299788	-1.341045	1.603628
H	-0.343781	-2.311470	1.569576
H	-0.997659	-2.020012	3.208345
H	-2.959984	-0.883767	2.345314
H	-2.764474	-2.261304	1.240635
H	1.947693	-0.502575	3.655358
H	3.619057	-0.465930	1.809182
H	-3.706960	-1.271280	-1.422441
H	-2.001294	-1.478519	-3.228431

TS_{3H}

E = -3334.096291 au

Ni	0.007389	0.007279	0.007845
S	-0.008071	0.024171	2.180369
S	2.176950	0.024171	0.122329
S	-2.135956	-0.023906	-0.005476
S	0.122264	-0.023906	-2.132461
C	1.456963	0.895940	2.531191
C	2.439535	0.895940	1.605720
C	-2.521918	0.047373	-1.688757
C	-1.534924	0.047373	-2.618393
C	1.150534	-2.002421	2.251233
C	2.178402	-2.002421	1.283099
H	1.418593	-1.925788	3.300503
H	0.244809	-2.563952	2.043008
H	2.024712	-2.563952	0.366543
H	3.209765	-1.925789	1.613424
H	1.579219	1.316631	3.526094
H	3.425347	1.316631	1.787254
H	-3.575090	0.092908	-1.955881
H	-1.738590	0.092908	-3.685654

3H

E = -3334.123629 au

Ni	0.010610	-0.006851	0.012309
S	-0.004962	-0.003953	2.267344
S	2.242852	-0.003840	0.332200
S	-2.118110	-0.087766	-0.100113
S	0.215968	-0.087622	-2.109466
C	1.271401	1.230552	2.499982
C	2.283053	1.230640	1.629004
C	-2.449636	-0.170813	-1.816826
C	-1.432358	-0.170753	-2.692577
C	1.099094	-1.485159	2.451359
C	2.260985	-1.484930	1.451494
H	1.452734	-1.507156	3.485209
H	0.429676	-2.333441	2.289051
H	2.200745	-2.333383	0.765530
H	3.230585	-1.506292	1.955283
H	1.191049	1.904319	3.347925
H	3.133458	1.904485	1.675620
H	-3.494319	-0.216495	-2.113749
H	-1.570637	-0.216391	-3.769799

4H

E = -3334.105618 au

Ni	0.006291	0.015783	0.000503
S	-0.001335	0.027783	2.228546
S	2.223267	-0.026496	0.008177
S	-1.643916	1.496244	0.043594
S	0.073598	0.155306	-2.222198
C	1.638581	-0.308012	2.615511
C	2.593149	-0.385295	1.647077
C	-2.119652	1.586571	-1.604760
C	-1.345503	1.051509	-2.589359
C	-1.360092	-1.554226	-0.042131
C	-0.065185	-2.062978	-0.085626
H	-1.912236	-1.532744	0.893043
H	-1.938068	-1.438060	-0.953660
H	0.375813	-2.366499	-1.030754
H	0.414818	-2.427760	0.817129
H	1.868801	-0.486323	3.664338
H	3.616547	-0.673915	1.877206
H	-3.059389	2.087511	-1.827371
H	-1.610234	1.142311	-3.641266

5H

E = -3334.119314 au

Ni	0.005846	0.008105	0.011192
S	-0.000441	0.002471	2.272918
S	2.238527	0.004627	-0.034217
S	-2.037569	0.755086	0.008762
S	-0.013699	-0.269771	-2.115386
C	1.708085	-0.186386	2.647175
C	2.608919	-0.167182	1.641174
C	-2.566501	0.392841	-1.602096
C	-1.678669	-0.024958	-2.530338
C	-0.599760	-1.737226	1.868742
C	-0.394244	-1.890990	0.391914
H	-0.031713	-2.429758	2.495065
H	-1.655597	-1.736733	2.150271
H	-1.276097	-2.171899	-0.179644
H	0.499555	-2.435797	0.095091
H	1.975651	-0.257987	3.696790
H	3.669074	-0.259242	1.879173
H	-3.626643	0.504681	-1.815400
H	-1.962084	-0.257331	-3.554535

BMK/6-31++G**

1H

E = -3254.491686 au

Ni	0.000000	-0.000430	0.000000
S	-0.013208	-0.000067	2.175603
S	2.173481	0.000027	-0.096966
S	-2.173481	-0.000546	0.096966
S	0.013208	-0.000459	-2.175603
C	1.653871	-0.000232	2.552341
C	2.614128	-0.000189	1.554371
C	-2.614128	-0.001182	-1.554370
C	-1.653870	-0.001145	-2.552341
H	1.938997	-0.000355	3.604531
H	3.676516	-0.000279	1.798772
H	-3.676516	-0.001604	-1.798772
H	-1.938997	-0.001537	-3.604531

TS_{2yH}

E = -3332.975294 au

Ni	-0.017165	-0.012082	0.018768
S	0.017156	-0.060416	2.165676
S	2.170208	0.068638	-0.095974
S	-1.795895	-1.191668	-0.220861
S	-0.443340	1.146936	-1.792126
C	1.696194	-0.324745	2.562753
C	2.613690	-0.246794	1.551011
C	-2.687983	-0.373392	-1.478365
C	-2.060617	0.636110	-2.155722
C	-1.737139	-1.568226	2.937509
C	-2.761508	-1.598446	1.981159
H	-1.136040	-2.458837	3.108266
H	-1.805195	-0.864157	3.760070
H	-3.520556	-0.819018	1.983098
H	-3.044117	-2.549353	1.542002
H	1.973424	-0.430159	3.609539
H	3.680289	-0.322868	1.767971
H	-3.664960	-0.760544	-1.760070
H	-2.550593	1.118079	-3.003143

2yH

E = -3333.044953 au

Ni	0.001396	0.000765	-0.001534
S	-0.006855	0.004147	2.219390
S	2.218941	0.077346	-0.012201
S	-1.947857	-1.062479	-0.051623
S	-0.416033	0.898831	-1.987160
C	1.615533	-0.654342	2.605374
C	2.535066	-0.485290	1.625582
C	-2.906104	-0.044404	-1.174129
C	-2.162821	0.686852	-2.038367
C	-1.337476	-1.250729	2.586367
C	-2.533237	-0.844988	1.706207
H	-0.969906	-2.254191	2.343910
H	-1.596293	-1.191970	3.648825
H	-2.826972	0.198451	1.866782
H	-3.388376	-1.506879	1.879104
H	1.840361	-0.909182	3.637121
H	3.582045	-0.691950	1.856509
H	-3.969095	-0.243376	-1.276370
H	-2.671556	1.184935	-2.866197

2H

E = -3333.051750 au

Ni	0.008952	-0.025274	-0.005716
S	-0.013656	0.025510	2.261536
S	2.221978	-0.052602	-0.063957
S	-2.240803	-0.119845	0.189136
S	-0.082972	-0.575899	-2.146405
C	1.690764	-0.364522	2.642814
C	2.582688	-0.332418	1.624909
C	-2.692793	-1.009534	-1.302508
C	-1.757021	-1.086337	-2.274154
C	-0.905962	-1.621690	2.187647
C	-2.305718	-1.354267	1.605183
H	-0.317973	-2.289023	1.549694
H	-0.973428	-2.031973	3.201978
H	-2.969245	-0.912093	2.354964
H	-2.753637	-2.276287	1.219962
H	1.952938	-0.473403	3.691341
H	3.638792	-0.487359	1.857743
H	-3.741847	-1.263513	-1.427989
H	-2.046495	-1.496769	-3.244196

TS_{3H}

E = -3332.988165 au

Ni	0.007950	-0.019434	0.008441
S	-0.017034	0.055776	2.211536
S	2.208597	0.055776	0.115246
S	-2.162705	-0.063129	0.011681
S	0.140990	-0.063129	-2.158136
C	1.457231	0.929968	2.539449
C	2.447762	0.929968	1.606482
C	-2.529745	0.049318	-1.693688
C	-1.539379	0.049318	-2.626501
C	1.161055	-2.058542	2.256949
C	2.183479	-2.058542	1.293942
H	1.413292	-1.950421	3.308878
H	0.226885	-2.570108	2.036771
H	2.019559	-2.570108	0.348278
H	3.218441	-1.950421	1.608634
H	1.587912	1.361928	3.530919
H	3.429643	1.361928	1.796219
H	-3.581073	0.119522	-1.970603
H	-1.752928	0.119522	-3.692506

3H

E = -3333.033129 au

Ni	0.007238	0.029630	0.008374
S	-0.005024	0.027817	2.299461
S	2.274671	0.028021	0.336992
S	-2.149374	-0.074407	-0.084688
S	0.235941	-0.074190	-2.138105
C	1.302846	1.255909	2.538381
C	2.316293	1.255998	1.665959
C	-2.461583	-0.198718	-1.829839

C	-1.443360	-0.198625	-2.706383
C	1.083794	-1.494633	2.443282
C	2.255103	-1.494535	1.434943
H	1.439642	-1.538994	3.476811
H	0.392623	-2.322890	2.257196
H	2.173934	-2.322727	0.723701
H	3.224226	-1.538870	1.940524
H	1.226534	1.925926	3.392469
H	3.172164	1.926098	1.717581
H	-3.504878	-0.267918	-2.133620
H	-1.588603	-0.267744	-3.783259

4H

E = -3332.988094 au

Ni	0.062632	0.158770	0.005556
S	0.064942	0.232246	2.235386
S	2.244998	-0.213144	0.001743
S	-1.787173	1.374558	0.039163
S	0.164633	0.350038	-2.214931
C	1.659444	-0.346755	2.637431
C	2.593198	-0.567451	1.675220
C	-2.243148	1.455460	-1.643951
C	-1.386632	1.038798	-2.613084
C	-1.311367	-1.413090	-0.045366
C	-0.004736	-1.927055	-0.072635
H	-1.868356	-1.396850	0.889589
H	-1.871777	-1.303235	-0.971120
H	0.436234	-2.237698	-1.017986
H	0.457757	-2.285376	0.844347
H	1.855151	-0.552572	3.689835
H	3.574408	-0.985158	1.897382
H	-3.240188	1.833004	-1.867508
H	-1.644766	1.086222	-3.671070

5H

E = -3333.013366 au

Ni	0.027910	0.056353	0.022880
S	0.009331	0.046164	2.287989
S	2.266741	0.014169	-0.027978
S	-2.054896	0.727259	0.045752
S	0.022116	-0.221069	-2.111998
C	1.737248	-0.206535	2.672011
C	2.638716	-0.198082	1.666218
C	-2.583005	0.317355	-1.583659
C	-1.683672	-0.064868	-2.514946
C	-0.622370	-1.695086	1.838725
C	-0.412582	-1.827846	0.348976
H	-0.055755	-2.401645	2.452753
H	-1.681206	-1.675205	2.113276
H	-1.299380	-2.080464	-0.231949
H	0.479921	-2.375005	0.045858
H	1.991029	-0.304383	3.724726
H	3.697089	-0.329138	1.901699
H	-3.650781	0.381065	-1.787294
H	-1.963814	-0.320488	-3.536388

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1H

E = -3254.877043 au

Ni	0.000000	-0.000303	0.000000
S	-0.006712	-0.000311	2.146207
S	2.144357	-0.000222	-0.089343
S	-2.144357	-0.000787	0.089343
S	0.006712	-0.000699	-2.146207
C	1.643507	-0.000206	2.535866
C	2.597267	-0.000166	1.544649
C	-2.597266	-0.001152	-1.544649
C	-1.643507	-0.001113	-2.535866
H	1.917898	-0.000174	3.588298
H	3.659482	-0.000101	1.778315
H	-3.659482	-0.001418	-1.778315
H	-1.917898	-0.001346	-3.588297

TS_{2yH}

E = -3333.335496 au

Ni	-0.012138	-0.008544	0.013271
S	0.005005	-0.017089	2.125243
S	2.143657	-0.015495	-0.087609
S	-1.737251	-1.202268	-0.231263
S	-0.487334	1.181408	-1.723358
C	1.643120	-0.341522	2.549942
C	2.569097	-0.296550	1.550971
C	-2.672722	-0.383232	-1.424210
C	-2.075166	0.644236	-2.091018
C	-1.701575	-1.488360	2.893825
C	-2.693357	-1.605305	1.911444
H	-1.086849	-2.351885	3.130070
H	-1.846237	-0.776390	3.697384
H	-3.494950	-0.873319	1.879514
H	-2.936721	-2.590414	1.532140
H	1.904150	-0.448286	3.598521
H	3.630479	-0.387145	1.775624
H	-3.647704	-0.779031	-1.692178
H	-2.577649	1.128249	-2.926752

2yH

E = -3333.385956 au

Ni	-0.012808	-0.006927	0.014218
S	-0.009316	-0.016061	2.172096
S	2.169251	0.006989	-0.020769
S	-1.914445	-1.025512	-0.038655
S	-0.428397	0.935584	-1.909778
C	1.577444	-0.650545	2.584006
C	2.500118	-0.494399	1.607226
C	-2.877794	-0.053492	-1.141915
C	-2.143349	0.687582	-2.002848
C	-1.328043	-1.238032	2.566385
C	-2.512177	-0.841176	1.692373
H	-0.973336	-2.247767	2.339267
H	-1.582513	-1.169158	3.627358
H	-2.819423	0.194255	1.866857
H	-3.362569	-1.508261	1.856671
H	1.805187	-0.879309	3.619231
H	3.549219	-0.672593	1.841255
H	-3.933257	-0.272883	-1.259216
H	-2.643032	1.163249	-2.846171

2H

E = -3333.390363 au

Ni	-0.009666	-0.015836	0.013853
S	-0.010069	-0.008149	2.244333
S	2.169999	-0.018601	-0.061981
S	-2.219419	-0.140472	0.186750
S	-0.075108	-0.568435	-2.093882
C	1.664446	-0.393534	2.609744
C	2.550049	-0.330066	1.591872
C	-2.654844	-1.025120	-1.272991
C	-1.717941	-1.087926	-2.240677
C	-0.913473	-1.616012	2.181143
C	-2.296492	-1.333975	1.601644
H	-0.341320	-2.300297	1.550083
H	-0.990255	-2.026625	3.193521
H	-2.950545	-0.875781	2.348031
H	-2.766081	-2.252865	1.241727
H	1.940647	-0.509734	3.651827
H	3.608809	-0.474548	1.808396
H	-3.699408	-1.280488	-1.415564

H	-1.994764	-1.488832	-3.215846

TS_{3H}

E = -3333.341713 au

Ni	0.010154	0.008252	0.010780
S	-0.009517	0.034685	2.179086
S	2.175755	0.034685	0.120809
S	-2.130620	-0.028804	0.000729
S	0.128139	-0.028804	-2.126764
C	1.454986	0.895683	2.528997
C	2.437463	0.895683	1.603616
C	-2.512298	0.041315	-1.678709
C	-1.525469	0.041315	-2.608189
C	1.146476	-2.003190	2.243948
C	2.171373	-2.003190	1.278613
H	1.411488	-1.923612	3.293475
H	0.234812	-2.553402	2.032609
H	2.014930	-2.553402	0.355941
H	3.203174	-1.923612	1.605912
H	1.581800	1.311727	3.525022
H	3.424121	1.311727	1.789765
H	-3.564410	0.086065	-1.949066
H	-1.732426	0.086065	-3.674585

3H

E = -3333.372482 au

Ni	0.011976	-0.005803	0.013887
S	-0.005248	-0.002681	2.265037
S	2.240651	-0.002490	0.331636
S	-2.114452	-0.087575	-0.094014
S	0.221519	-0.087339	-2.104949
C	1.270281	1.226812	2.497729
C	2.280945	1.226901	1.627688
C	-2.440830	-0.173870	-1.807556
C	-1.424420	-0.173768	-2.682539
C	1.094074	-1.479289	2.444199
C	2.254498	-1.479177	1.445270
H	1.448629	-1.504188	3.477503
H	0.424825	-2.327386	2.280665
H	2.192444	-2.327238	0.759086
H	3.223572	-1.503977	1.949576
H	1.192103	1.899482	3.346412
H	3.131748	1.899653	1.676646
H	-3.484304	-0.221554	-2.107479
H	-1.565821	-0.221363	-3.759017

4H

E = -3333.349343 au

Ni	0.013438	0.033938	0.001147
S	0.000463	0.043424	2.222234
S	2.223220	-0.036462	0.009408
S	-1.650693	1.488990	0.041749
S	0.082788	0.167543	-2.214893
C	1.631422	-0.317523	2.610559
C	2.585378	-0.405740	1.644320
C	-2.127967	1.566197	-1.603460
C	-1.346847	1.039404	-2.585179
C	-1.350694	-1.532308	-0.040443
C	-0.057084	-2.040478	-0.085725
H	-1.900343	-1.510630	0.896198
H	-1.928206	-1.412576	-0.951853
H	0.382258	-2.342076	-1.032243
H	0.425018	-2.402324	0.817141
H	1.857919	-0.502916	3.658624
H	3.603616	-0.710282	1.875162
H	-3.074758	2.052056	-1.827895
H	-1.613676	1.122476	-3.636851

5H

E = -3333.365181 au

Ni	0.011327	0.022546	0.013811
S	0.001516	0.008491	2.269453
S	2.237207	0.009194	-0.032927
S	-2.034818	0.746374	0.018114
S	-0.006100	-0.255085	-2.107543
C	1.704740	-0.196547	2.642852
C	2.605082	-0.177919	1.638420
C	-2.562771	0.370792	-1.586860
C	-1.673153	-0.036832	-2.515645
C	-0.605076	-1.718171	1.858070
C	-0.392010	-1.871226	0.383690
H	-0.047281	-2.417669	2.485851
H	-1.663340	-1.710939	2.129986
H	-1.270533	-2.150163	-0.194031
H	0.504072	-2.414241	0.090712
H	1.972249	-0.276367	3.691577
H	3.663912	-0.281004	1.876531
H	-3.624527	0.467535	-1.797877
H	-1.957853	-0.276217	-3.537532

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1H

E = -3254.940766 au

Ni	0.000000	0.000000	0.000011
S	1.453461	-1.525031	0.000004
S	1.453461	1.525031	-0.000035
S	-1.453461	-1.525031	0.000007
S	-1.453461	1.525031	-0.000033
C	2.913745	-0.684013	-0.000372
C	2.913745	0.684013	-0.000389
C	-2.913745	-0.684013	-0.000366
C	-2.913745	0.684013	-0.000384
H	3.836361	-1.257474	-0.000597
H	3.836361	1.257474	-0.000629
H	-3.836361	-1.257474	-0.000589
H	-3.836361	1.257474	-0.000621

TS_{2yH}

E = -3333.433521 au

Ni	0.000119	0.439415	-0.000082
S	1.391471	-0.914320	0.716251
S	1.512067	1.821200	-0.568670
S	-1.391283	-0.914459	-0.716342
S	-1.511945	1.821186	0.568247
C	2.915870	-0.325878	0.200813
C	2.940920	0.911367	-0.348567
C	-2.915679	-0.326214	-0.200534
C	-2.940725	0.911107	0.348622
C	0.679216	-3.176132	0.117812
C	-0.679646	-3.175911	-0.117962
H	1.369234	-3.321017	-0.707722
H	1.048601	-3.426724	1.104285
H	-1.369630	-3.320742	0.707615
H	-1.048996	-3.426719	-1.104409
H	3.808027	-0.900879	0.424858
H	3.879765	1.386011	-0.623648
H	-3.807822	-0.901304	-0.424396
H	-3.879567	1.385682	0.623828

2yH

E = -3333.522341 au

Ni	-0.024955	-0.012448	0.027392
S	-0.011390	-0.031647	2.161490
S	2.133927	-0.017376	-0.012617
S	-1.943034	-0.947231	-0.018246

S	-0.390182	0.890947	-1.899493
C	1.551931	-0.711868	2.568869
C	2.467862	-0.567455	1.597894
C	-2.873874	0.049813	-1.119186
C	-2.116196	0.743728	-1.983466
C	-1.352070	-1.192390	2.560999
C	-2.526367	-0.750251	1.692098
H	-1.044348	-2.215095	2.328762
H	-1.603613	-1.120381	3.620972
H	-2.793244	0.292914	1.879545
H	-3.398015	-1.384877	1.863800
H	1.769390	-0.980263	3.595790
H	3.511407	-0.784888	1.817459
H	-3.941651	-0.107721	-1.213658
H	-2.594114	1.244494	-2.823288

2H

E = -3333.528052 au

Ni	0.030303	-0.390276	-0.349534
S	1.404024	1.323536	-0.436564
S	1.644462	-1.765277	0.047865
S	-1.562143	1.088834	-0.617599
S	-1.385528	-1.911575	0.226423
C	2.883119	0.660422	0.228886
C	2.938669	-0.672350	0.367657
C	-2.921108	0.345630	0.210282
C	-2.810512	-0.963994	0.465866
C	0.507329	2.055789	0.972232
C	-0.902409	2.390745	0.488037
H	0.486165	1.321717	1.780343
H	1.023810	2.956896	1.313239
H	-0.906564	3.320621	-0.084231
H	-1.583685	2.503510	1.333102
H	3.726478	1.326880	0.365654
H	3.869300	-1.130110	0.699588
H	-3.839759	0.914280	0.297362
H	-3.674802	-1.503876	0.849055

TS_{3H}

E = -3333.447048 au

Ni	-0.249107	0.000000	-0.238322
S	1.268019	1.487480	-0.436348
S	1.268020	-1.487480	-0.436348
S	-1.684174	1.526567	0.002583
S	-1.684174	-1.526567	0.002583
C	2.496133	0.679080	-1.284302
C	2.496133	-0.679080	-1.284302
C	-3.171557	0.670162	0.188219
C	-3.171557	-0.670162	0.188219
C	2.149547	0.691019	1.691403
C	2.149547	-0.691019	1.691403
H	3.081671	1.233459	1.572908
H	1.341221	1.223914	2.182198
H	1.341221	-1.223914	2.182198
H	3.081671	-1.233459	1.572908
H	3.318039	1.259506	-1.693487
H	3.318039	-1.259506	-1.693487
H	-4.076648	1.259847	0.298868
H	-4.076648	-1.259847	0.298868

3H

E = -3333.512100 au

Ni	-0.311138	-0.000019	-0.080544
S	1.372561	1.470611	-0.071592
S	1.372621	-1.470544	-0.071634
S	-1.770383	1.520816	-0.011707
S	-1.770297	-1.520937	-0.011782
C	2.379279	0.663638	-1.294768
C	2.379280	-0.663491	-1.294814
C	-3.286973	0.665697	0.064834
C	-3.286936	-0.665906	0.064803
C	2.204963	0.766519	1.390549
C	2.205213	-0.766471	1.390407
H	3.219209	1.168078	1.432381
H	1.644405	1.159874	2.240882
H	1.645104	-1.160161	2.240881
H	3.219601	-1.167716	1.431791
H	2.971820	1.273661	-1.968635
H	2.971823	-1.273469	-1.968721
H	-4.192410	1.263434	0.107362
H	-4.192339	-1.263697	0.107306

4H

E = -3333.457160 au

Ni	-0.000007	0.000033	-0.076069
S	-1.568737	-1.504318	-0.259670
S	-1.427482	1.562516	-0.476613
S	1.427461	-1.562381	-0.476920
S	1.568726	1.504411	-0.259434
C	-3.007879	-0.565145	-0.280528
C	-2.952525	0.773604	-0.363648
C	2.952510	-0.773495	-0.363803
C	3.007869	0.565236	-0.280445
C	0.474765	-0.519656	1.821925
C	-0.474763	0.519418	1.822021
H	0.149065	-1.535031	2.028956
H	1.519422	-0.288158	2.006289
H	-0.149057	1.534759	2.029214
H	-1.519416	0.287891	2.006367
H	-3.948886	-1.102765	-0.202420
H	-3.836488	1.403885	-0.345471
H	3.836469	-1.403785	-0.345740
H	3.948876	1.102841	-0.202240

5H

E = -3333.489222 au

Ni	0.080481	0.133467	-0.221540
S	-1.564216	-1.354690	-0.388400
S	-1.336947	1.810837	-0.275899
S	1.484363	-1.384343	-0.764310
S	1.606526	1.504546	0.264886
C	-2.995218	-0.348639	-0.271931
C	-2.845492	0.981205	-0.234200
C	2.980805	-0.737499	-0.185773
C	3.034710	0.529560	0.239282
C	-1.030375	-1.568531	1.364168
C	-0.074194	-0.437699	1.623438
H	-1.918846	-1.566431	1.997942
H	-0.533733	-2.539590	1.402673
H	0.901346	-0.729845	2.005139
H	-0.493906	0.413499	2.154427
H	-3.956556	-0.849989	-0.288043
H	-3.729675	1.614182	-0.180364
H	3.844128	-1.395824	-0.185346
H	3.947539	0.993790	0.601474

M05/6-31++G**

1H

E = -3255.733850 au

Ni	0.000000	0.000210	0.000000
S	-0.008679	0.000033	2.151224
S	2.149294	0.000114	-0.091502
S	-2.149294	-0.000453	0.091502
S	0.008679	-0.000355	-2.151223
C	1.644184	-0.000306	2.536731
C	2.598157	-0.000271	1.545292

C	-2.598157	-0.001257	-1.545292
C	-1.644184	-0.001213	-2.536731
H	1.918164	-0.000534	3.589803
H	3.660997	-0.000470	1.778522
H	-3.660997	-0.001788	-1.778522
H	-1.918164	-0.001707	-3.589803

TS_{2yH}

E = -3334.419568 au

Ni	0.000000	0.000000	0.000000
S	0.000000	0.000000	2.140226
S	2.187266	0.000000	-0.076236
S	-1.739202	-1.224253	-0.238642
S	-0.499667	1.187929	-1.768927
C	1.648384	-0.345837	2.574193
C	2.583664	-0.292535	1.582677
C	-2.696038	-0.391624	-1.428724
C	-2.102570	0.631185	-2.108688
C	-1.670266	-1.492919	2.872486
C	-2.686441	-1.573840	1.890989
H	-1.072628	-2.376185	3.077188
H	-1.823451	-0.828950	3.714449
H	-3.468343	-0.820279	1.887755
H	-2.983937	-2.555050	1.541786
H	1.899784	-0.464635	3.623556
H	3.641740	-0.385305	1.821626
H	-3.675480	-0.785307	-1.682070
H	-2.616961	1.106664	-2.942085

2yH

E = -3334.262813 au

Ni	-0.009752	-0.005271	0.010829
S	-0.003793	-0.009572	2.168185
S	2.179184	0.012317	-0.020048
S	-1.909366	-1.026259	-0.046500
S	-0.428802	0.935414	-1.921065
C	1.577231	-0.666139	2.579925
C	2.503816	-0.500689	1.603756
C	-2.880856	-0.039671	-1.134202
C	-2.143764	0.695648	-2.003019
C	-1.332291	-1.226261	2.573822
C	-2.512782	-0.855575	1.690318
H	-0.969057	-2.236995	2.373760
H	-1.587533	-1.132216	3.631893
H	-2.846010	0.171406	1.857104
H	-3.349660	-1.540932	1.843386
H	1.801502	-0.888206	3.618071
H	3.552712	-0.677695	1.839867
H	-3.935291	-0.267081	-1.251711
H	-2.644726	1.169324	-2.846779

2H

E = -3334.267523 au

Ni	-0.012441	-0.013892	0.015841
S	-0.007939	-0.002736	2.250659
S	2.174507	-0.013283	-0.063999
S	-2.225710	-0.143124	0.185092
S	-0.076942	-0.547702	-2.105085
C	1.668105	-0.403322	2.609060
C	2.552585	-0.333896	1.586535
C	-2.651482	-1.040653	-1.273992
C	-1.713654	-1.084874	-2.245903
C	-0.919655	-1.612328	2.186741
C	-2.299291	-1.335328	1.606279
H	-0.346032	-2.300003	1.563740
H	-0.994465	-2.014733	3.201622
H	-2.955849	-0.873752	2.347035
H	-2.767977	-2.253317	1.246775
H	1.945113	-0.517118	3.651768
H	3.611613	-0.479921	1.800898
H	-3.696496	-1.296442	-1.417828
H	-1.989425	-1.480874	-3.223256

TS_{3H}

E = -3334.423120 au

Ni	-0.000134	-0.001245	-0.000143
S	0.000005	-0.000685	2.209340
S	2.205386	-0.000685	0.132124
S	-2.164998	-0.022674	-0.016478
S	0.113019	-0.022674	-2.162108
C	1.463688	0.904436	2.538396
C	2.446324	0.904436	1.612865
C	-2.543853	0.061139	-1.712452
C	-1.557265	0.061139	-2.641705
C	1.158684	-2.009414	2.266930
C	2.193584	-2.009414	1.292173
H	1.434425	-1.945284	3.314347
H	0.263207	-2.586804	2.061598
H	2.042169	-2.586804	0.386020
H	3.222636	-1.945284	1.630056
H	1.579336	1.350130	3.522639
H	3.421890	1.350130	1.787163
H	-3.595939	0.114373	-1.980816
H	-1.762234	0.114373	-3.707957

3H

E = -3334.249050 au

Ni	0.009515	-0.004712	0.011032
S	-0.000956	-0.000887	2.280204
S	2.254982	-0.000813	0.338050
S	-2.117675	-0.086342	-0.105624
S	0.210418	-0.086236	-2.109862
C	1.273098	1.227834	2.502781
C	2.285602	1.227922	1.631037
C	-2.452323	-0.174632	-1.819680
C	-1.434831	-0.174591	-2.695632
C	1.101225	-1.482817	2.448702
C	2.258125	-1.482532	1.453313
H	1.452467	-1.510106	3.481728
H	0.426034	-2.324072	2.283155
H	2.195837	-2.324056	0.761243
H	3.227184	-1.508930	1.954786
H	1.194518	1.901749	3.350933
H	3.135956	1.901908	1.679405
H	-3.498222	-0.221800	-2.112368
H	-1.568764	-0.221736	-3.773423

4H

E = -3334.224222 au

Ni	0.008322	0.020925	0.000682
S	0.002877	0.046246	2.230634
S	2.225843	-0.041978	0.008973
S	-1.656308	1.486772	0.041922
S	0.083149	0.171776	-2.223056
C	1.636318	-0.309252	2.615571
C	2.590077	-0.399509	1.646350
C	-2.127109	1.574066	-1.604966
C	-1.344702	1.049060	-2.589545
C	-1.354585	-1.536628	-0.039763
C	-0.057163	-2.046249	-0.086795
H	-1.904696	-1.521997	0.895868
H	-1.936250	-1.425296	-0.948561
H	0.377690	-2.353354	-1.032749
H	0.422304	-2.416913	0.812851
H	1.863254	-0.491586	3.664387
H	3.609342	-0.702069	1.876529
H	-3.073325	2.062024	-1.828566

H	-1.609784	1.134677	-3.641763

5H

E = -3334.239397 au

Ni	0.006439	0.013361	0.017053
S	0.000026	0.008052	2.273644
S	2.244964	0.007972	-0.033913
S	-2.043528	0.751371	0.011937
S	-0.010229	-0.260589	-2.110986
C	1.705893	-0.193076	2.643887
C	2.607937	-0.171272	1.636358
C	-2.565536	0.383175	-1.596000
C	-1.673677	-0.027451	-2.525150
C	-0.601272	-1.728775	1.860492
C	-0.397219	-1.887031	0.390540
H	-0.030464	-2.415320	2.488829
H	-1.654842	-1.725369	2.145013
H	-1.278773	-2.161462	-0.182987
H	0.496875	-2.430151	0.094215
H	1.970774	-0.271735	3.693899
H	3.666729	-0.269155	1.877704
H	-3.627137	0.483671	-1.808685
H	-1.954318	-0.263662	-3.549198

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1H

E = -3255.540711 au

Ni	0.000000	0.000000	0.000266
S	1.488783	-1.562313	0.000003
S	1.488783	1.562313	-0.000042
S	-1.488783	-1.562313	0.000002
S	-1.488783	1.562313	-0.000034
C	2.946953	-0.686821	-0.000396
C	2.946953	0.686821	-0.000416
C	-2.946953	-0.686821	-0.000392
C	-2.946953	0.686821	-0.000407
H	3.877095	-1.254198	-0.000630
H	3.877095	1.254198	-0.000667
H	-3.877095	-1.254198	-0.000628
H	-3.877095	1.254198	-0.000654

TS_{2yH}

E = -3334.023180 au

Ni	0.000047	0.470129	-0.000043
S	1.398925	-0.939930	0.754097
S	1.571298	1.864148	-0.555015
S	-1.398881	-0.939885	-0.754176
S	-1.571154	1.864191	0.554964
C	2.931922	-0.361196	0.198304
C	2.974670	0.891059	-0.332911
C	-2.931848	-0.361117	-0.198337
C	-2.974549	0.891134	0.332897
C	0.693265	-3.112884	0.092077
C	-0.693458	-3.112813	-0.092027
H	1.343635	-3.255281	-0.768046
H	1.093559	-3.444646	1.044309
H	-1.343843	-3.255055	0.768113
H	-1.093782	-3.444658	-1.044219
H	3.821324	-0.952008	0.405942
H	3.930951	1.348148	-0.590649
H	-3.821270	-0.951903	-0.405960
H	-3.930814	1.348235	0.590678

2yH

E = -3334.073443 au

Ni	-0.015151	-0.007534	0.016641
S	-0.005642	0.003753	2.190845
S	2.176519	-0.049448	-0.027379
S	-1.955879	-0.986189	-0.039813
S	-0.397956	0.940469	-1.922910
C	1.561710	-0.713139	2.580031
C	2.484068	-0.583769	1.601160
C	-2.886177	0.049812	-1.127580
C	-2.128773	0.761858	-1.990713
C	-1.364986	-1.191792	2.572247
C	-2.533791	-0.761034	1.703154
H	-1.027150	-2.208086	2.336998
H	-1.613889	-1.126712	3.636275
H	-2.800921	0.290678	1.860867
H	-3.412382	-1.390885	1.875519
H	1.784448	-0.958544	3.614735
H	3.527456	-0.809558	1.829078
H	-3.952499	-0.127344	-1.237223
H	-2.617541	1.265466	-2.826817

2H

E = -3334.079451 au

Ni	0.032054	-0.390048	-0.371252
S	1.432952	1.364850	-0.471399
S	1.669978	-1.782680	0.045322
S	-1.598057	1.115580	-0.661533
S	-1.393421	-1.929687	0.252613
C	2.902361	0.672940	0.221410
C	2.951746	-0.666761	0.371711
C	-2.934902	0.352203	0.214188
C	-2.813353	-0.961011	0.487132
C	0.488595	2.033599	0.980282
C	-0.898687	2.406669	0.483529
H	0.454487	1.250854	1.746319
H	1.019562	2.908424	1.374903
H	-0.877103	3.338480	-0.091484
H	-1.603131	2.523986	1.313176
H	3.751729	1.336736	0.356004
H	3.881337	-1.119492	0.723882
H	-3.862672	0.912880	0.293737
H	-3.676326	-1.496121	0.889123

TS_{3H}

E = -3334.031277 au

Ni	-0.278323	0.000000	-0.188615
S	1.288475	1.514708	-0.339591
S	1.288475	-1.514708	-0.339591
S	-1.744783	1.559975	0.018842
S	-1.744783	-1.559975	0.018842
C	2.494785	0.674576	-1.267967
C	2.494785	-0.674576	-1.267967
C	-3.228935	0.676206	0.143936
C	-3.228935	-0.676206	0.143936
C	2.202673	0.702310	1.665801
C	2.202673	-0.702310	1.665801
H	3.144992	1.231840	1.549026
H	1.438271	1.223551	2.237462
H	1.438271	-1.223551	2.237462
H	3.144992	-1.231840	1.549026
H	3.287503	1.262671	-1.727632
H	3.287503	-1.262671	-1.727632
H	-4.146111	1.258815	0.217331
H	-4.146111	-1.258815	0.217331

3H

E = -3334.062335 au

Ni	-0.316313	0.000023	-0.116164
S	1.391472	1.499830	-0.112676
S	1.391869	-1.499565	-0.113238
S	-1.791370	1.546628	-0.015403

S	-1.790932	-1.547053	-0.015915
C	2.427122	0.666662	-1.313967
C	2.427503	-0.665690	-1.313997
C	-3.305810	0.669159	0.095036
C	-3.305622	-0.670056	0.094807
C	2.192943	0.762651	1.394360
C	2.191441	-0.762680	1.394940
H	3.207179	1.169582	1.454537
H	1.600116	1.166625	2.220884
H	1.595511	-1.164882	2.220103
H	3.204732	-1.171511	1.458235
H	3.040338	1.277802	-1.971962
H	3.041044	-1.276436	-1.972052
H	-4.213087	1.267666	0.154971
H	-4.212734	-1.268837	0.154503

4H

E = -3334.043931 au

Ni	-0.000006	0.000038	0.031780
S	-1.617484	-1.539612	-0.057713
S	-1.425189	1.552064	-0.685315
S	1.425134	-1.551860	-0.685660
S	1.617491	1.539683	-0.057480
C	-3.024001	-0.579176	-0.304506
C	-2.944462	0.759206	-0.524984
C	2.944430	-0.759078	-0.525137
C	3.023996	0.579260	-0.304404
C	0.458514	-0.519538	2.010473
C	-0.458496	0.519276	2.010574
H	0.131503	-1.548023	2.151230
H	1.521198	-0.323092	2.134140
H	-0.131484	1.547736	2.151509
H	-1.521179	0.322807	2.134216
H	-3.983327	-1.093145	-0.242946
H	-3.838394	1.376832	-0.605512
H	3.838347	-1.376712	-0.605771
H	3.983331	1.093195	-0.242724

5H

E = -3334.056066 au

Ni	0.091114	0.133848	-0.200078
S	-1.587759	-1.379880	-0.398185
S	-1.349719	1.845634	-0.296524
S	1.524684	-1.405249	-0.786825
S	1.656070	1.532007	0.275844
C	-3.008446	-0.341872	-0.278899
C	-2.852264	0.996666	-0.249101
C	3.023090	-0.732860	-0.221953
C	3.081859	0.542474	0.209212
C	-1.042653	-1.590026	1.400894
C	-0.121972	-0.451372	1.681234
H	-1.957367	-1.615070	2.001787
H	-0.534632	-2.559539	1.418919
H	0.865684	-0.715489	2.060464
H	-0.564741	0.406227	2.189183
H	-3.975736	-0.838445	-0.287633
H	-3.742409	1.627355	-0.199243
H	3.892309	-1.388490	-0.225463
H	4.003631	1.002085	0.563989

O3LYP/6-31++G**

1H

E = -3255.969989 au

Ni	0.000000	-0.000061	0.000000
S	0.003553	-0.000188	2.159328
S	2.157863	-0.000107	-0.079591
S	-2.157863	-0.000677	0.079591
S	-0.003553	-0.000582	-2.159328
C	1.659342	-0.000239	2.552094
C	2.614091	-0.000204	1.559847
C	-2.614091	-0.001196	-1.559847
C	-1.659341	-0.001152	-2.552093
H	1.930104	-0.000304	3.606032
H	3.677673	-0.000240	1.789828
H	-3.677673	-0.001564	-1.789828
H	-1.930104	-0.001484	-3.606032

TS_{2yH}

E = -3334.488480 au

Ni	0.005109	0.003596	-0.005586
S	0.002895	0.017307	2.110312
S	2.175237	-0.050257	-0.076504
S	-1.706581	-1.216560	-0.247559
S	-0.522654	1.213537	-1.730374
C	1.630564	-0.355853	2.563775
C	2.573245	-0.327087	1.575243
C	-2.688237	-0.388660	-1.407351
C	-2.111931	0.651814	-2.079628
C	-1.673949	-1.442546	2.868751
C	-2.656106	-1.605451	1.865584
H	-1.059059	-2.296632	3.138117
H	-1.872525	-0.740804	3.670842
H	-3.479719	-0.898288	1.824428
H	-2.889784	-2.611465	1.536106
H	1.870245	-0.474736	3.616545
H	3.630298	-0.431977	1.815807
H	-3.667483	-0.790370	-1.651506
H	-2.633712	1.133491	-2.905440

2yH

E = -3334.525431 au

Ni	-0.005333	-0.002880	0.005928
S	0.001813	-0.012625	2.158936
S	2.187839	-0.028647	-0.027218
S	-1.903708	-1.017110	-0.049743
S	-0.441875	0.973988	-1.908994
C	1.586086	-0.653949	2.586549
C	2.517334	-0.508358	1.609238
C	-2.883282	-0.048382	-1.147956
C	-2.154678	0.704728	-2.011389
C	-1.332747	-1.229959	2.578431
C	-2.518327	-0.855126	1.692363
H	-0.977041	-2.244658	2.380595
H	-1.586853	-1.131072	3.637411
H	-2.853652	0.170609	1.867597
H	-3.354161	-1.544143	1.842106
H	1.806545	-0.872644	3.626004
H	3.566455	-0.681223	1.848892
H	-3.936630	-0.280642	-1.263753
H	-2.657024	1.173637	-2.857406

2H

E = -3334.527715 au

Ni	-0.004547	-0.018537	0.007780
S	0.003566	-0.019675	2.240874
S	2.186975	-0.003119	-0.064109
S	-2.214639	-0.153164	0.177764
S	-0.078707	-0.561697	-2.114188
C	1.681909	-0.402790	2.609187
C	2.571574	-0.320124	1.590078
C	-2.658862	-1.032559	-1.287428
C	-1.723566	-1.080461	-2.263974
C	-0.926310	-1.625057	2.206136
C	-2.306791	-1.342337	1.609474
H	-0.359030	-2.332590	1.598695
H	-1.015329	-2.008848	3.228507

H	-2.966977	-0.873187	2.343400
H	-2.776041	-2.263443	1.255696
H	1.956954	-0.516016	3.652337
H	3.633098	-0.447879	1.805955
H	-3.705433	-1.281896	-1.428380
H	-2.003278	-1.463917	-3.245820

TS_{3H}

E = -3334.488531 au

Ni	0.001701	0.005715	0.001805
S	0.000602	0.000532	2.184402
S	2.180457	0.000532	0.131229
S	-2.149037	-0.013523	-0.022822
S	0.105731	-0.013523	-2.146556
C	1.459219	0.893631	2.533812
C	2.442016	0.893631	1.608129
C	-2.539412	0.059713	-1.705884
C	-1.550975	0.059713	-2.636879
C	1.158853	-1.999602	2.265858
C	2.192503	-1.999602	1.292277
H	1.433214	-1.929435	3.313950
H	0.265701	-2.583120	2.064113
H	2.044530	-2.583120	0.388660
H	3.222313	-1.929435	1.628823
H	1.572691	1.326199	3.524766
H	3.424411	1.326199	1.780657
H	-3.593483	0.107343	-1.969520
H	-1.751105	0.107343	-3.704830

3H

E = -3334.511091 au

Ni	0.005945	-0.013118	0.006884
S	0.001212	-0.013684	2.271783
S	2.246336	-0.013520	0.339001
S	-2.128287	-0.090455	-0.117717
S	0.200117	-0.090251	-2.122152
C	1.269594	1.229677	2.500057
C	2.283361	1.229766	1.627309
C	-2.465744	-0.160104	-1.833544
C	-1.446441	-0.160018	-2.711023
C	1.112766	-1.492934	2.467788
C	2.275097	-1.492779	1.467327
H	1.465557	-1.505041	3.501900
H	0.446343	-2.344520	2.312947
H	2.221422	-2.344400	0.785304
H	3.245180	-1.504595	1.970112
H	1.182370	1.908790	3.343312
H	3.130145	1.908959	1.666480
H	-3.511767	-0.198390	-2.126940
H	-1.581016	-0.198232	-3.789050

4H

E = -3334.500646 au

Ni	-0.008882	-0.022652	-0.000842
S	0.003120	-0.001808	2.242881
S	2.224389	-0.016270	0.011374
S	-1.637858	1.504567	0.041028
S	0.050509	0.137598	-2.238171
C	1.652425	-0.283460	2.625833
C	2.608284	-0.343150	1.651936
C	-2.101889	1.627927	-1.606733
C	-1.338586	1.079522	-2.597858
C	-1.380047	-1.602265	-0.042606
C	-0.083331	-2.111616	-0.088486
H	-1.931945	-1.582111	0.891942
H	-1.961823	-1.491472	-0.951254
H	0.356567	-2.416002	-1.033059
H	0.395884	-2.482684	0.810980
H	1.891771	-0.443731	3.675821
H	3.640189	-0.599671	1.883141
H	-3.025928	2.158156	-1.828309
H	-1.597590	1.189835	-3.649616

5H

E = -3334.510627 au

Ni	-0.007279	-0.024500	0.004857
S	-0.002121	-0.020403	2.275482
S	2.241038	-0.004622	-0.034549
S	-2.042105	0.775496	-0.016797
S	-0.035821	-0.298934	-2.132325
C	1.708976	-0.169552	2.649643
C	2.612477	-0.143494	1.641265
C	-2.570530	0.441155	-1.631304
C	-1.686721	0.000859	-2.558884
C	-0.586286	-1.774018	1.893087
C	-0.396143	-1.933164	0.414522
H	-0.002525	-2.454266	2.518058
H	-1.636979	-1.784935	2.192050
H	-1.283530	-2.218667	-0.144651
H	0.493903	-2.479537	0.111139
H	1.977506	-0.225294	3.700081
H	3.674145	-0.208861	1.882233
H	-3.626114	0.582471	-1.850559
H	-1.969248	-0.217181	-3.586694

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1H

E = -3255.700510 au

Ni	0.000000	0.000000	-0.000137
S	1.472998	-1.544474	-0.000036
S	1.472998	1.544474	-0.000074
S	-1.472998	-1.544474	-0.000031
S	-1.472998	1.544474	-0.000073
C	2.930793	-0.686466	-0.000355
C	2.930793	0.686466	-0.000371
C	-2.930793	-0.686466	-0.000347
C	-2.930793	0.686466	-0.000367
H	3.858400	-1.253578	-0.000540
H	3.858400	1.253578	-0.000569
H	-3.858400	-1.253578	-0.000529
H	-3.858400	1.253578	-0.000564

TS_{2yH}

E = -3334.224177 au

Ni	-0.000001	0.450947	-0.000003
S	1.406144	-0.934857	0.726830
S	1.542012	1.853210	-0.545055
S	-1.406149	-0.934856	-0.726832
S	-1.542011	1.853213	0.545050
C	2.932206	-0.334026	0.205065
C	2.961349	0.914027	-0.330332
C	-2.932209	-0.334024	-0.205063
C	-2.961349	0.914030	0.330333
C	0.689838	-3.166485	0.086807
C	-0.689835	-3.166487	-0.086808
H	1.336902	-3.309006	-0.774004
H	1.100598	-3.450329	1.047792
H	-1.336900	-3.309009	0.774003
H	-1.100595	-3.450329	-1.047793
H	3.827461	-0.907581	0.424143
H	3.907964	1.382402	-0.593524
H	-3.827464	-0.907578	-0.424137
H	-3.907963	1.382406	0.593527

2yH

E = -3334.297075 au

Ni	-0.008114	-0.004008	0.008926
S	-0.002588	-0.007330	2.185224
S	2.182263	-0.039761	-0.018744
S	-1.955944	-0.973606	-0.037468
S	-0.402781	0.931242	-1.932554
C	1.565649	-0.709401	2.582348
C	2.489866	-0.583830	1.608220
C	-2.887450	0.047411	-1.132821
C	-2.136179	0.761112	-1.996010
C	-1.357479	-1.188228	2.573463
C	-2.534810	-0.761348	1.694825
H	-1.032385	-2.207376	2.348297
H	-1.615368	-1.111297	3.631671
H	-2.809764	0.282915	1.865008
H	-3.401697	-1.401691	1.870030
H	1.781438	-0.969863	3.611443
H	3.528217	-0.815653	1.837593
H	-3.953623	-0.118092	-1.229398
H	-2.627783	1.266810	-2.824938

2H

E = -3334.311025 au

Ni	0.031275	-0.408173	-0.367548
S	1.423529	1.342002	-0.445364
S	1.671000	-1.788084	0.037138
S	-1.586069	1.105621	-0.632606
S	-1.407173	-1.938573	0.216832
C	2.896339	0.660703	0.232841
C	2.954403	-0.676923	0.368978
C	-2.932324	0.344864	0.214364
C	-2.822361	-0.969567	0.469965
C	0.506507	2.061101	0.971309
C	-0.905979	2.401572	0.485489
H	0.486187	1.320138	1.774411
H	1.020405	2.961746	1.320797
H	-0.905565	3.333111	-0.086309
H	-1.588810	2.514524	1.331026
H	3.740788	1.324800	0.379736
H	3.886491	-1.127308	0.710026
H	-3.853027	0.910025	0.311836
H	-3.688465	-1.500179	0.864740

TS_{3H}

E = -3334.236797 au

Ni	-0.263243	0.000000	-0.221444
S	1.293735	1.505062	-0.407980
S	1.293736	-1.505062	-0.407980
S	-1.715466	1.546144	0.009293
S	-1.715466	-1.546144	0.009293
C	2.501502	0.680071	-1.291266
C	2.501502	-0.680071	-1.291266
C	-3.204163	0.672132	0.173070
C	-3.204163	-0.672132	0.173070
C	2.171714	0.696610	1.694963
C	2.171714	-0.696610	1.694963
H	3.108750	1.232657	1.581883
H	1.374330	1.225242	2.208727
H	1.374330	-1.225242	2.208727
H	3.108750	-1.232657	1.581883
H	3.314383	1.256380	-1.725606
H	3.314383	-1.256379	-1.725606
H	-4.115460	1.256337	0.270528
H	-4.115460	-1.256337	0.270528

3H

E = -3334.293801 au

Ni	-0.328412	-0.000016	-0.090085
S	1.403324	1.490084	-0.078888
S	1.403327	-1.490034	-0.078855
S	-1.797682	1.540772	-0.014082
S	-1.797637	-1.540844	-0.014077
C	2.400262	0.665803	-1.305225
C	2.400202	-0.665776	-1.305273
C	-3.312246	0.667736	0.068695
C	-3.312227	-0.667851	0.068699
C	2.216030	0.768799	1.399885
C	2.216529	-0.768739	1.399635
H	3.231188	1.169016	1.453668
H	1.642893	1.163615	2.242393
H	1.644353	-1.164188	2.242498
H	3.231981	-1.168333	1.452457
H	2.988879	1.272088	-1.986822
H	2.988770	-1.272071	-1.986905
H	-4.222084	1.260305	0.114632
H	-4.222046	-1.260448	0.114650

4H

E = -3334.239964 au

Ni	-0.000008	0.000033	-0.071891
S	-1.590798	-1.520604	-0.241374
S	-1.446730	1.574954	-0.524130
S	1.446705	-1.574809	-0.524442
S	1.590786	1.520695	-0.241135
C	-3.026128	-0.569183	-0.292798
C	-2.968151	0.774593	-0.395460
C	2.968134	-0.774479	-0.395615
C	3.026116	0.569276	-0.292710
C	0.468853	-0.518048	1.886245
C	-0.468845	0.517800	1.886343
H	0.144335	-1.540656	2.057418
H	1.521547	-0.298113	2.036426
H	-0.144322	1.540379	2.057676
H	-1.521536	0.297840	2.036512
H	-3.972221	-1.099610	-0.213813
H	-3.858009	1.398543	-0.385797
H	3.857987	-1.398437	-0.386065
H	3.972210	1.099687	-0.213623

5H

E = -3334.269897 au

Ni	0.087957	0.138714	-0.217582
S	-1.582956	-1.368364	-0.387114
S	-1.350964	1.829993	-0.285465
S	1.507505	-1.392211	-0.776336
S	1.632772	1.524844	0.261519
C	-3.010093	-0.346107	-0.275286
C	-2.859186	0.988557	-0.243600
C	3.005113	-0.733152	-0.197051
C	3.060091	0.538294	0.229419
C	-1.041662	-1.579622	1.378425
C	-0.082483	-0.450359	1.644099
H	-1.934919	-1.574583	2.007408
H	-0.549251	-2.554058	1.414539
H	0.895460	-0.742293	2.021147
H	-0.502090	0.404293	2.170587
H	-3.974392	-0.843286	-0.289928
H	-3.747173	1.618293	-0.194636
H	3.871111	-1.389423	-0.194389
H	3.975899	0.998474	0.591865

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1H

E = -3255.70450208 au

Ni	0.000000	0.000000	0.000270
S	1.480312	-1.552479	0.000021
S	1.480312	1.552479	-0.000025
S	-1.480312	-1.552479	0.000018

S	-1.480312	1.552479	-0.000016
C	2.940065	-0.686315	-0.000395
C	2.940065	0.686315	-0.000417
C	-2.940065	-0.686315	-0.000393
C	-2.940065	0.686315	-0.000407
H	3.867687	-1.251927	-0.000647
H	3.867687	1.251927	-0.000685
H	-3.867687	-1.251927	-0.000646
H	-3.867687	1.251927	-0.000671

TS_{2yH}

E = -3334.22961186 au

Ni	0.000001	0.465778	0.000002
S	1.403538	-0.925877	0.746181
S	1.557377	1.850614	-0.576598
S	-1.403534	-0.925876	-0.746180
S	-1.557377	1.850612	0.576603
C	2.934047	-0.341274	0.206864
C	2.972110	0.900029	-0.346732
C	-2.934045	-0.341275	-0.206866
C	-2.972110	0.900027	0.346731
C	0.688546	-3.148606	0.103986
C	-0.688550	-3.148604	-0.103985
H	1.355160	-3.292322	-0.740447
H	1.073844	-3.438937	1.072829
H	-1.355164	-3.292318	0.740448
H	-1.073849	-3.438936	-1.072828
H	3.824650	-0.920228	0.426547
H	3.921384	1.356545	-0.616992
H	-3.824647	-0.920228	-0.426553
H	-3.921384	1.356543	0.616990

2yH

E = -3334.29707520 au

Ni	-0.000024	-0.521252	-0.001235
S	1.337503	0.997961	-0.800908
S	1.670563	-1.926688	0.182355
S	-1.337751	1.002198	0.790001
S	-1.670429	-1.927917	-0.176852
C	2.917913	0.501228	-0.196410
C	3.006609	-0.810111	0.105908
C	-2.918084	0.501947	0.188200
C	-3.006614	-0.811079	-0.106753
C	0.761196	2.514831	0.063870
C	-0.761564	2.514371	-0.083043
H	1.067146	2.478551	1.112739
H	1.196755	3.394365	-0.414609
H	-1.067503	2.472351	-1.131702
H	-1.197198	3.396467	0.390627
H	3.763291	1.167001	-0.321086
H	3.987967	-1.237705	0.302441
H	-3.763545	1.168304	0.309140
H	-3.987911	-1.239898	-0.300901

2H

E = -3334.30339686 au

Ni	0.031480	-0.409365	-0.363003
S	1.426442	1.341951	-0.454885
S	1.676905	-1.790339	0.051497
S	-1.585202	1.105446	-0.641947
S	-1.410552	-1.935781	0.245638
C	2.905095	0.663010	0.221926
C	2.963245	-0.674752	0.369429
C	-2.942315	0.347354	0.197884
C	-2.831776	-0.964770	0.471378
C	0.507287	2.059313	0.975737
C	-0.906634	2.400695	0.496911
H	0.492417	1.313913	1.773481
H	1.025043	2.957294	1.323658
H	-0.915017	3.337069	-0.064864
H	-1.589651	2.492899	1.343575
H	3.748198	1.329213	0.359098
H	3.895634	-1.122621	0.709990
H	-3.863342	0.912603	0.278497
H	-3.700107	-1.491730	0.863663

TS_{3H}

E = -3334.24020984 au

Ni	-0.267333	0.000000	-0.222349
S	1.292806	1.508019	-0.394868
S	1.292806	-1.508019	-0.394868
S	-1.724765	1.553186	0.011002
S	-1.724765	-1.553186	0.011002
C	2.510585	0.677631	-1.285123
C	2.510585	-0.677631	-1.285123
C	-3.211706	0.673818	0.170904
C	-3.211706	-0.673818	0.170904
C	2.173303	0.699462	1.682174
C	2.173303	-0.699462	1.682174
H	3.112605	1.230315	1.573153
H	1.385088	1.223099	2.212587
H	1.385088	-1.223099	2.212587
H	3.112605	-1.230315	1.573153
H	3.317825	1.257743	-1.721924
H	3.317825	-1.257743	-1.721924
H	-4.124373	1.254679	0.266163
H	-4.124373	-1.254680	0.266163

3H

E = -3334.28526505 au

Ni	-0.321026	0.000004	-0.124440
S	1.404650	1.492492	-0.108421
S	1.404942	-1.492322	-0.108794
S	-1.794585	1.546358	-0.021636
S	-1.794286	-1.546668	-0.021958
C	2.430242	0.666391	-1.316992
C	2.430493	-0.665725	-1.317028
C	-3.308293	0.668305	0.094289
C	-3.308165	-0.668937	0.094146
C	2.194282	0.768577	1.397050
C	2.193444	-0.768584	1.397369
H	3.206842	1.170115	1.466745
H	1.599525	1.164434	2.222495
H	1.596905	-1.163479	2.221992
H	3.205470	-1.171164	1.468817
H	3.033811	1.274161	-1.982176
H	3.034279	-1.273220	-1.982265
H	-4.216685	1.259621	0.159049
H	-4.216444	-1.260441	0.158759

4H

E = -3334.24528229 au

Ni	-0.000008	0.000034	-0.049979
S	-1.600941	-1.527861	-0.200086
S	-1.447669	1.571100	-0.576826
S	1.447629	-1.570934	-0.577175
S	1.600933	1.527946	-0.199853
C	-3.032173	-0.571892	-0.297124
C	-2.969178	0.772363	-0.431438
C	2.969153	-0.772249	-0.431595
C	3.032162	0.571977	-0.297023
C	0.465958	-0.516987	1.927367
C	-0.465942	0.516743	1.927471
H	0.143081	-1.541280	2.086094
H	1.520550	-0.302935	2.066189
H	-0.143060	1.541009	2.086355

H	-1.520530	0.302666	2.066290
H	-3.980744	-1.096013	-0.217742
H	-3.859794	1.393968	-0.440687
H	3.859759	-1.393867	-0.440952
H	3.980736	1.096074	-0.217519

5H

E = -3334.26967116 au

Ni	0.087165	0.136975	-0.207845
S	-1.585188	-1.370535	-0.386315
S	-1.355472	1.833930	-0.289292
S	1.515368	-1.388637	-0.797219
S	1.641445	1.527604	0.275903
C	-3.015139	-0.346187	-0.284700
C	-2.864469	0.990086	-0.253895
C	3.013406	-0.729670	-0.214039
C	3.069494	0.540073	0.225064
C	-1.043792	-1.580387	1.396650
C	-0.085848	-0.453806	1.663160
H	-1.943343	-1.571826	2.014804
H	-0.556355	-2.556316	1.429283
H	0.892985	-0.747068	2.034486
H	-0.504979	0.399147	2.190926
H	-3.977610	-0.844592	-0.301573
H	-3.752335	1.618996	-0.211497
H	3.879434	-1.384507	-0.216294
H	3.985974	0.994725	0.590014

Reference

[S1] (a) Hohne, E.; Prokop, P.; Hoyer, E. *c. Chem.*,**1966**, *6,* 71. (b) Smith, A. E.; Abstracts, American Crystallographic Association Meeting, Minneapolis, Minn., **Aug** 1967. (c) Browall, K. W.; Bursh, T.; Interrante, L. V.; Kasper, J. S. *Inorg. Chem.* **1972**, *11*, 1800. (a) and (b) are cited by Kasper in (c).

[S2] Lim, B.S.; Fomitchev, D.V.; Holm, R. H.; *Inorg. Chem.* **2001**, *40*, 4257.

[S3] Sartain, D.; Truter, M. R.; *J. Chem. Soc. (A)* **1967**, 1264.

[S4] Wang, K.; Patil, A. O.; Zushma, S.; McConnachie, J. M. *J. Inorg. Biochem.* **2007**, *101*, 1883.