

Supporting Information

Internal Coulombic Assistance in Intermolecular Frustrated Lewis Pairs Activation of Dihydrogen

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Table S1. Reaction energies values with the zero-point vibrational term corrected (kcal/mol) calculated (CCSD(T)/def2-TZVPP//B3LYP-D4/def2-TZVP) relative to species **3**.

	E	X	Y	1+2	4+5^{a)}
3^Ca	CH ₂	Me	F	18.06	43.07
3^Cb		Me	CF ₃	33.76	61.47
3^Cc		NH ₂	F	19.34	53.12
3^Cd		NH ₂	CF ₃	32.99	69.48
3^Ce		Tms	F	26.83	30.18
3^Cf		Tms	CF ₃	41.30	47.36
3^{Si}a	SiH ₂	Me	F	-1.98	-6.38
3^{Si}b		Me	CF ₃	18.67	13.37
3^{Si}c		NH ₂	F	1.50	-2.38
3^{Si}d		NH ₂	CF ₃	21.18	16.40
3^{Si}e		Tms	F	0.66	-8.74
3^{Si}f		Tms	CF ₃	20.13	9.84
3^Na	NH	Me	F	18.88	101.76
3^Nb		Me	CF ₃	29.31	115.69
3^Nc		NH ₂	F	16.90	110.02
3^Nd		NH ₂	CF ₃	28.41	125.03
3^Ne		Tms	F	28.33	82.33
3^Nf		Tms	CF ₃	34.90	92.39
3^Pa	PH	Me	F	-2.82	29.24
3^Pb		Me	CF ₃	9.52	41.13
3^Pc		NH ₂	F	-3.11	33.54
3^Pd		NH ₂	CF ₃	11.49	47.71
3^Pe		Tms	F	1.39	21.47
3^Pf		Tms	CF ₃	11.98	31.63
3^Oa	O	Me	F	1.05	133.09
3^Ob		Me	CF ₃	20.57	10.83
3^Oc		NH ₂	F	9.08	152.25
3^Od		NH ₂	CF ₃	20.04	21.45
3^Oe		Tms	F	15.51	113.93
3^Of		Tms	CF ₃	29.36	-13.99
3^Sa	S ^{b)}	Me	F	2.99	84.37
3^Sb		Me	CF ₃	-1.09	6.27
3^Sc		NH ₂	F	3.65	90.48
3^Sd		NH ₂	CF ₃	3.76	16.58
3^Se		Tms	F	-4.72	58.55
3^Sf		Tms	CF ₃	5.82	-4.91

^a **5'** stands for Y-E-SiY₃

^b **3^S** correspond to compounds **1^S·2a-f**

Table S2. Computed (B3LYP-D4/def2-TZVP) P-Si distance (Å), Löwdin atomic charges (in brackets) and WBI (parenthesis) data in species **3**.

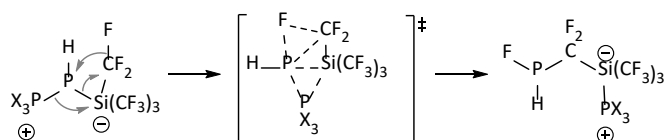
X	Y	E		
		CH ₂	SiH ₂	NH
Me	F	3.055	3.494	3.065
		[0.76/-0.43] (0.000)	[0.68/-0.53] (0.014)	[0.66/-0.48] (0.006)
Me	CF ₃	3.312	3.881	3.240
		[0.76/0.20] (0.008)	[0.69/0.11] (0.009)	[0.58/0.14] (0.012)
NH ₂	F	2.994	3.418	3.046
		[0.46/-0.42] (0.014)	[0.40/-0.53] (0.019)	[0.39/-0.49] (0.006)
NH ₂	CF ₃	3.240	3.765	3.182
		[0.47/0.20] (0.009)	[0.40/0.10] (0.012)	[0.37/0.15] (0.011)
Tms	F	3.213	3.762	3.115
		[0.61/-0.41] (0.005)	[0.49/-0.52] (0.004)	[0.58/-0.34] (0.009)
Tms	CF ₃	3.452	4.189	3.432
		[0.57/0.31] (0.010)	[0.50/0.11] (0.008)	[0.51/0.16] (0.0161)
X	Y	E		
		PH	O	S
Me	F	3.446	2.979	4.214
		[0.59/-0.56] (0.012)	[0.61/-0.50] (0.006)	[0.35/-0.35] (0.001)
Me	CF ₃	3.696	3.207	3.548
		[0.51/-0.09] (0.010)	[0.61/0.17] (0.012)	[0.13/-0.24] (0.007)
NH ₂	F	3.287	3.168	4.089
		[0.30/-0.56] (0.020)	[0.28/-0.47] (0.003)	[-0.21/-0.83] (0.001)
NH ₂	CF ₃	3.514	3.156*	4.108
		[0.30/0.10] (0.015)	[0.27/0.13] (0.011)	[-0.24/-0.14] (0.004)
Tms	F	3.643	3.015	3.558
		[0.44/-0.59] (0.007)	[0.51/-0.53] (0.009)	[0.16/ -0.97] (0.006)
Tms	CF ₃	4.165	3.271*	4.213
		[0.41/0.17] (0.005)	[0.35/0.04] (0.021)	[0.06/-0.24] (0.004)

* Almost linear P-E-Si arrangement

Table S3. E-Si bond distances for 1,3-zwitterionic dipoles Me₃P-E-SiF₄ (**3**) and their simplified HE-SiF₄ counterparts (in parenthesis), homolytic (left) and heterolytic (right) Bond Dissociation Energies (BDE) for **3** and sum of (Mulliken) electric charge (a.u.) at the SiF₄ group.

	d_{E-Si}^a	BDE ^b	$\Sigma q_{SiF_4}^M$
3^Ca	1.954 (1.900)	99.66/200.30	-0.556
3^{Si}a	2.402 (2.379)	67.78/176.58	-0.532
3^Na	1.804 (1.730)	96.55/229.54	-0.531
3^Pa	2.357 (2.305)	63.09/176.93	-0.504
3^Oa	1.803 (1.686)	67.39/245.86	-0.471
3^Sa	3.422 (2.211)	4.89/258.95	-0.049

^a Å; ^b kcal/mol



Scheme S1. Triple concerted shift in Si-CF₃-substituted PH-bridged zwitterionic species **3^P**.

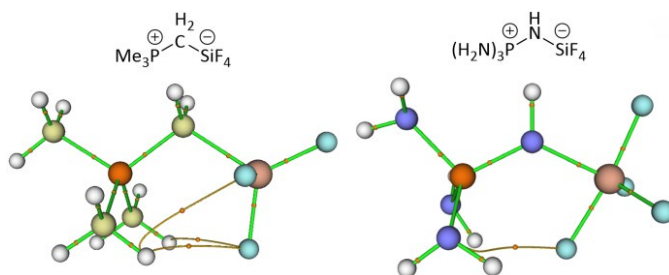


Figure S1. Computed (B3LYP/def2-TZVP) structures for dipolar molecules **3** with short P-Si contacts (**3^Ca** and **3^Nc**), showing BCPs (small orange spheres) and bond paths.

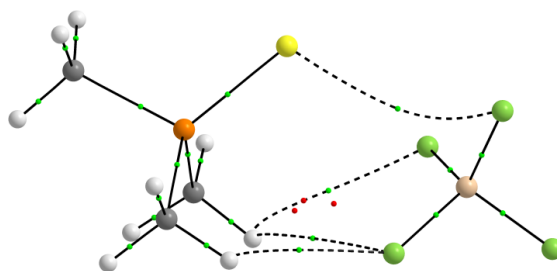


Figure S2. Peripheral noncovalent interactions in the encounter complex between Me₃P=S and SiF₄.

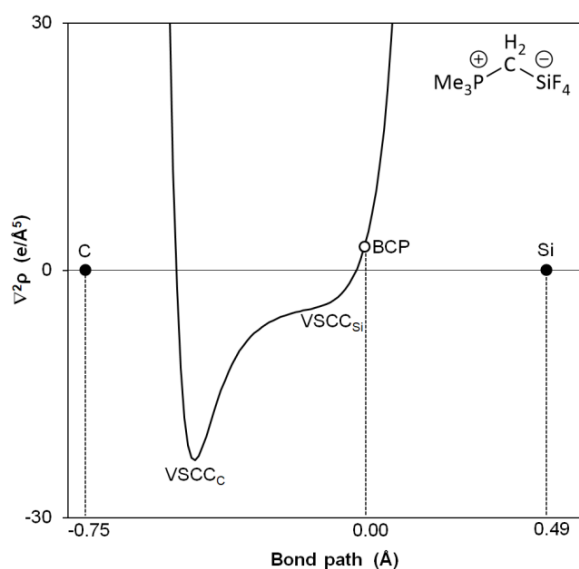


Figure S3. Computed (B3LYP-D3/def2-TZVPPecp) representation of the Laplacian of electron density $\nabla^2\rho$ variation along the C-Si bond path for **3^ca**.

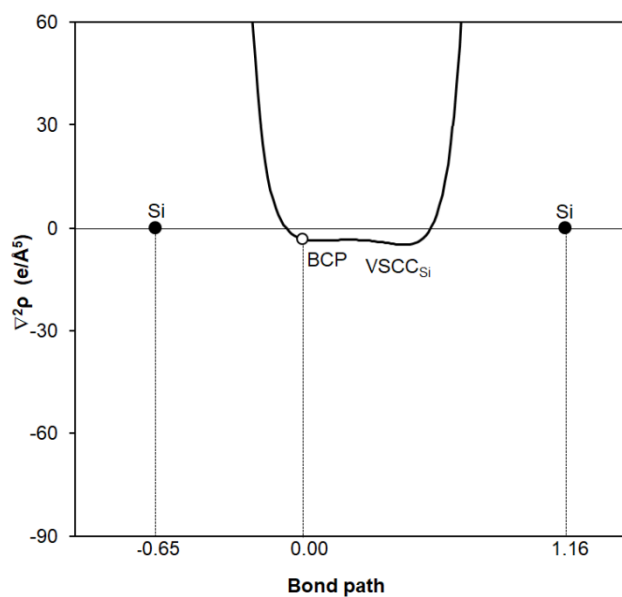


Figure S4. Computed (B3LYP-D3/def2-TZVPPecp) representation of the Laplacian of electron density $\nabla^2\rho$ variation along the Si-Si bond path for **3^{Si}a**.

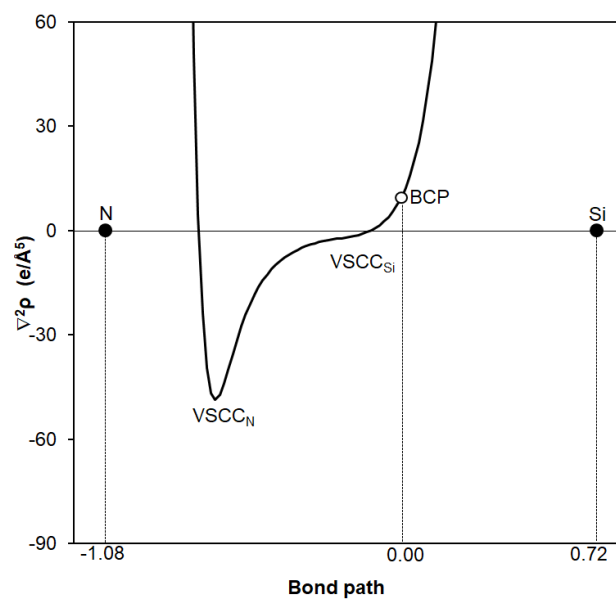


Figure S5. Computed (B3LYP-D3/def2-TZVPPecp) representation of the Laplacian of electron density $\nabla^2\rho$ variation along the N-Si bond path for **3^{Na}**.

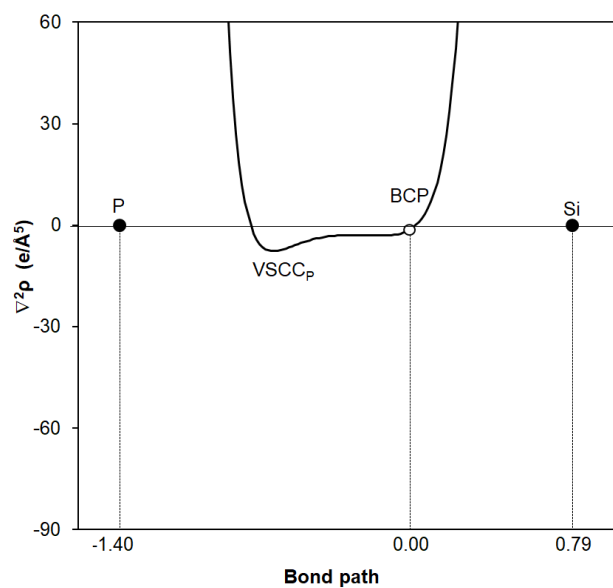


Figure S6. Computed (B3LYP-D3/def2-TZVPPecp) representation of the Laplacian of electron density $\nabla^2\rho$ variation along the P-Si bond path for **3^{Pa}**.

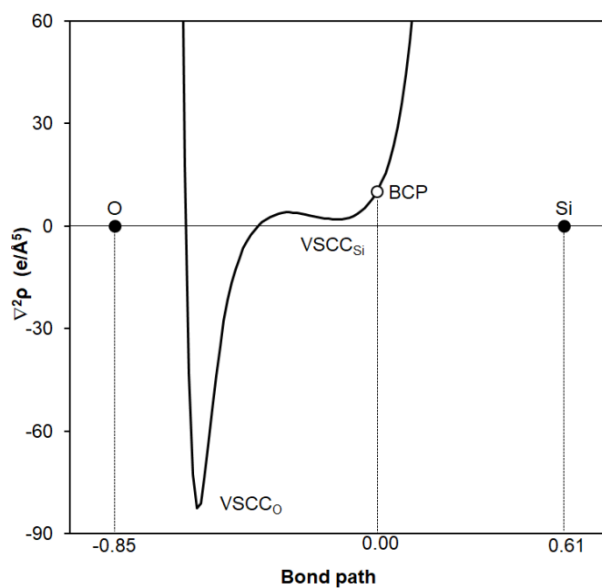


Figure S7. Computed (B3LYP-D3/def2-TZVPPecp) representation of the Laplacian of electron density $\nabla^2\rho$ variation along the O–Si bond path for **3^oa**.

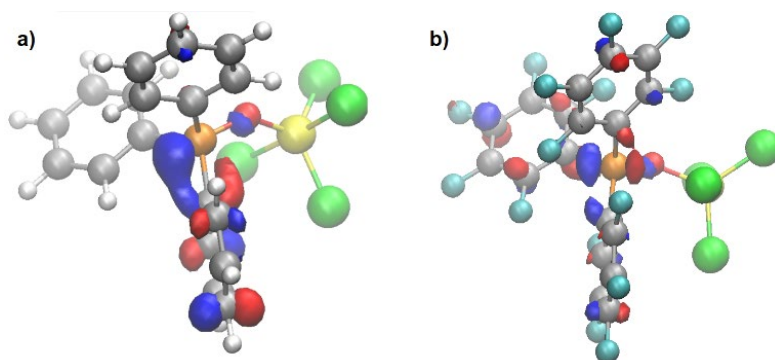


Figure S8. Computed (PWPB95-D3/def2-TZVPP//PBEh-3c) Kohn–Sham isosurfaces (0.07 au) for LUMO in (a) **3^{oh}** and (b) **3^{oj}**.

Experimental Section

DFT calculations were performed with the ORCA program.^[1] All geometry optimizations were run in redundant internal coordinates in the gas phase, with tight convergence criteria, and using the B3LYP^[2] functional together with the RIJCOSX algorithm,^[3] the 2010 Grimme's semiempirical atom-pair-wise London dispersion correction (DFT-D4)^[4] and the Ahlrichs segmented def2-TZVP basis set.^[5] Only for those molecules that participate in the H₂ activation reaction (Figure 1) the optimization has been carried out with the faster and computationally less expensive Grimme's functional PBEh-3c.^[6] Harmonic frequency calculations verified the nature of ground states or TS having all real (positive) frequencies or only one imaginary (negative) frequency, respectively. From these optimized geometries, all reported data were obtained by means of single-point (SP) calculations using the more polarized def2-TZVPP^[7] basis set. Reported energies were corrected for the zero-point vibrational term at the optimization level and obtained by means of the recently developed near-linear scaling domain-based local pair natural orbital (DLPNO) method^[8] to achieve coupled cluster theory with single, double, and perturbative triple excitations (CCSD(T)).^[9] Properties derived from the topological analysis of the electronic density were obtained with the Multiwfn program,^[10] whereas Figure 2 and was drawn with Visual Molecular Dynamics (VMD).^[11]

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Calculated structures

Cartesian coordinates (in Å), G correction (G-E) and ZPE (in hartrees) for TSs and minima were computed at B3LYP-D4/def2-TZVP. For TSs the imaginary frequency is given. In addition, electronic energies (in hartrees) are quoted using, unless otherwise indicated, the default DLPNO-CCSD(T)/def2-TZVPP(ecp) level and for those molecules corresponding to the energy profile (Figure 1) at the DLPNO-CCSD(T)/def2-TZVPP(ecp)//PBEh-3c level (indicated).

1^ca (Me₃P=CH₂) E = -499.619588986455 au

ZPE = 0.13658274 au

G = 0.10566015 au

P	-3.85323603672128	1.39762638486176	0.00190958042454
C	-4.66800320780442	1.56271291046078	1.64010109409087
H	-4.28528830424310	2.46179130618256	2.12674039132370
H	-5.75506619059520	1.63717503702862	1.56433131582664
H	-4.39581154719651	0.70515520050243	2.25512248752701
C	-4.66514957948196	2.76712647691078	-0.91283970410972
H	-4.40092749873157	2.68866002850379	-1.96722529625343
H	-5.75138915264151	2.76347344485826	-0.79914186463234
H	-4.27365866699687	3.71367754008254	-0.53560960945712
C	-4.54139219076527	-0.12136789371683	-0.71241458842354
H	-5.63093779010343	-0.09507770366906	-0.69128383274909
H	-4.20512427967447	-0.22158668203652	-1.74369123251365
H	-4.19277837096755	-0.98043930122725	-0.14016062667239
C	-2.19507016121103	1.34818405535866	-0.02354674402858
H	-1.69993775130447	0.47429643268638	-0.41666485327917
H	-1.59620749156128	2.16224709321304	0.35623582292628

1^cb ((NH₂)₃P=CH₂) E = -547.778618967859 au

ZPE = 0.10599803 au

G = 0.07600506 au

P	-4.06302406789984	1.39752183049951	0.01523449464953
C	-2.43340583212944	1.20749784664072	0.16500867113134
H	-1.89337384477797	0.68564061467671	-0.61140497574430
H	-1.87744480200177	1.83805971275235	0.84325619773817
N	-4.68360902741050	1.72955155152851	1.53181309565415
H	-5.64107219638335	2.03766663072154	1.60782421849147
H	-4.40450222881094	1.10512364330563	2.27246481557992
N	-4.85289858900376	0.09478370827920	-0.69987045477842
H	-4.50620532566980	-0.80998987168148	-0.41499814718108
H	-4.95152335928278	0.16138057886258	-1.70258651361037
N	-4.74570594071798	2.59445756886433	-0.97212088945545

H	-5.74871453275934	2.73187699787433	-0.96270341418818
H	-4.24211444315240	3.46878361767603	-0.95679159828681

1^c (Tms₃P=CH₂) E = -1605.944359611334 au
 ZPE = 0.36098181 au
 G = 0.30948811 au

P	0.15400583085553	0.28666032169297	-0.01196195795053
Si	-0.11307757832182	2.56817401983145	-0.30989599365034
Si	-1.49524156560981	-0.41718870506135	1.39038427037284
Si	-0.14114582234416	-0.72046685946760	-2.02815928998049
C	0.62551054689940	3.36670242247037	1.22043628608226
H	0.76157121771476	4.44002233302368	1.06347169327798
H	-0.00606395171631	3.23336208627319	2.09986075024227
H	1.60138909228766	2.92800933636370	1.43872907714448
C	0.93419107411879	3.04648834997583	-1.79895621319589
H	0.51581918015149	2.67824129884546	-2.73696991547810
H	1.01111685397813	4.13462344707334	-1.87411666101066
H	1.94642683633511	2.64866892532523	-1.69943230570937
C	-1.89077983920599	3.14760615692607	-0.55662214119422
H	-1.91406024127581	4.22596843979956	-0.73996310541418
H	-2.36643546820441	2.65660260587564	-1.40717747259020
H	-2.49979168258541	2.95342901851655	0.32836211050194
C	-1.50774172730222	0.13232389275148	-2.99846468881207
H	-1.25732851146885	1.16820332544742	-3.23101069173855
H	-1.66577687825257	-0.38859556107472	-3.94686550048165
H	-2.45502350204962	0.12749575212287	-2.45688486964979
C	1.49664922909715	-0.58813043740002	-2.92982408193818
H	1.44419373428298	-1.11819066954566	-3.88477449971211
H	1.77066393878307	0.44767345281296	-3.13328046569838
H	2.29031357695558	-1.04155009732785	-2.33385586196482
C	-0.56292403435289	-2.52518373164395	-1.74516092228189
H	-1.57194468764230	-2.65883560928456	-1.35210238814308
H	-0.49886664563938	-3.07412917886020	-2.68863272930834
H	0.14478612506832	-2.96918947003195	-1.04359447785896
C	-1.49339410035432	0.71894895469380	2.88623709498932
H	-1.81129674250167	1.73108919513387	2.63183698409901
H	-2.18150282300128	0.33558098869373	3.64484036506070
H	-0.50062982685682	0.77894783863297	3.33575587971435
C	-3.16168353957470	-0.33060676400449	0.52585605362584
H	-3.22341972816868	-1.04266980335460	-0.29886709445684
H	-3.95756399869798	-0.57745217179313	1.23411622837384
H	-3.36822328608142	0.66462780545735	0.13031637397997
C	-1.09011163533445	-2.16617801015103	1.91482605266663

H	-1.72519854210515	-2.46713276707766	2.75261962069142
H	-1.24036839619028	-2.87670654694638	1.10183454703529
H	-0.04507739995804	-2.23292565206487	2.22057437703241
C	1.65355253033340	-0.31071400266923	0.60645219546940
H	1.82639205229762	-0.11954147775879	1.66238768091643
H	2.51924062563737	-0.11168175222150	-0.01858571305773

1^{Si}a (Me₃P=SiH₂) E = -750.655268432920 au

ZPE = 0.12887738 au

G = 0.09582512 au

P	-3.92254188618552	1.30484970326826	0.06627470405057
C	-4.74208728792121	1.55457075693400	1.67720053515410
H	-4.35884840058013	2.46683776598157	2.13532568530603
H	-5.82475110752205	1.63464175185137	1.56742680329284
H	-4.50410640899521	0.71751708897969	2.33339989447553
C	-4.56132143341437	2.67266921997873	-0.96524308414794
H	-4.17676717865589	2.55731288058945	-1.97840293574820
H	-5.65359183161253	2.68960846985910	-0.98814195426394
H	-4.18974360177283	3.61652574934436	-0.56685889803047
C	-4.72976748610551	-0.17719029925108	-0.62742790275635
H	-5.81263456960749	-0.05457665506695	-0.68102575879876
H	-4.33908316435613	-0.36050953553834	-1.62869449143664
H	-4.49196572187764	-1.03918694865681	-0.00434330795627
Si	-1.66008058028155	1.01390606422821	0.30117256170483
H	-1.56520160251968	1.15424881112306	-1.21510179360128
H	-1.57748595859202	2.51242950637532	0.57630228275594

1^{Si}b ((NH₂)₃P=SiH₂) E = -798.798960298222 au

ZPE = 0.09609601 au

G = 0.06346256 au

P	-4.17252916264605	1.34441453030106	0.07221777924965
Si	-1.95193880539796	0.96762694981009	0.46306556052486
H	-1.78320108272829	0.93344278032037	-1.04863329057276
H	-1.77515961105997	2.47753229111089	0.58747170398368
N	-4.93421928301863	1.53360484272020	1.54024710570670
H	-5.93692622491366	1.49343861601284	1.63601019815476
H	-4.40930172090646	1.34202926984616	2.37720569642340
N	-5.10191855862932	0.13084961342281	-0.65575756105805
H	-5.09152635780903	-0.74580934929703	-0.15110200053010
H	-4.88104858643415	-0.01648317847151	-1.63214882260250
N	-4.55471142958625	2.57970995742299	-0.98313298837172

H	-5.52452501465517	2.83361759037821	-1.11916827881766
H	-3.92658835221494	3.36838051642287	-0.97114960209027

1^{Si}c (Tms₃P=SiH₂) E = -1857.006729478627 au

ZPE = 0.35340856 au

G = 0.30110941 au

P	0.08865737771938	0.26875111684144	-0.05557661135467
Si	-0.03936826523921	2.52760075329578	-0.28928862306300
Si	-1.54654721954703	-0.42473843325519	1.35792568508218
Si	-0.22382043414665	-0.70475803562882	-2.08370924816670
C	0.71077417551636	3.29665240574111	1.24127168962093
H	0.78282551965857	4.38027143615351	1.11218934188305
H	0.11587728084607	3.10255320639205	2.13409873292431
H	1.71245525714644	2.90042878820991	1.41217665061450
C	0.98422329019223	2.98364812948307	-1.79318035257612
H	0.54310264570419	2.62165455566386	-2.72277560957440
H	1.06458204139160	4.07176068152961	-1.86508817899828
H	1.99347549048735	2.57741581140031	-1.70808117270031
C	-1.81837773173128	3.09624206059366	-0.51278357219687
H	-1.84403172692150	4.17953766922179	-0.66220263373351
H	-2.29062589632435	2.62875545770742	-1.37783766489118
H	-2.42570860450202	2.87289195274543	0.36590807554610
C	-1.60283098147669	0.14357114795843	-3.03627871293485
H	-1.36299482470262	1.18535535700865	-3.25386492425489
H	-1.75604517088779	-0.36552778378473	-3.99201994335882
H	-2.54741633053498	0.11999304172957	-2.49095635685358
C	1.40288647138472	-0.56803492629716	-2.99993978757286
H	1.33692055179800	-1.09298579295985	-3.95699666232559
H	1.67759798373913	0.46755564284623	-3.20069496169949
H	2.20614819571315	-1.02315326880984	-2.41733086747524
C	-0.63583430467524	-2.51139105789610	-1.79911470810752
H	-1.61588157474662	-2.64998092296505	-1.34076629206851
H	-0.63951750608731	-3.03995529133786	-2.75639666926026
H	0.11497937763583	-2.97886373694496	-1.15978311204715
C	-1.56772413277576	0.74832911675495	2.82007862731383
H	-1.92071137630768	1.74423714633897	2.54916606984838
H	-2.23870310654376	0.35720806091954	3.59014607205698
H	-0.57246613452723	0.84277083021106	3.25681916845582
C	-3.21927725146293	-0.41820555297732	0.50223622223743
H	-3.25937785073886	-1.13866889851894	-0.31625251080545
H	-3.99977156440200	-0.68963580245794	1.21885022358341
H	-3.46478030152102	0.56553265087453	0.09973899131682
C	-1.09520304229691	-2.14796073179606	1.93160730696300

H	-1.81964846571975	-2.49177513498945	2.67557846849359
H	-1.08691360370740	-2.86542472837493	1.11099396952320
H	-0.10459569138766	-2.15755737933586	2.38903376837415
Si	2.15932372004215	-0.54276826250297	0.76065055539471
H	1.88859218761213	0.15510869411452	2.09071159901594
H	2.86690181632698	0.65594072709759	0.13547655777098

1^Na (Me₃P=NH) E = -515.701004908343 au

ZPE = 0.12718839 au

G = 0.09630599 au

P	-3.83875667932864	1.34127367976327	-0.02366978126071
N	-2.29912766556626	1.11479265285512	-0.12633064734217
H	-1.69098696804624	1.84772164350300	0.21389653266511
C	-4.56992691742749	1.54023676304060	1.64351464307756
H	-4.17570596974730	2.44917740699155	2.10154637702120
H	-5.65941434054023	1.60489907513779	1.61215210441948
H	-4.27466280543243	0.69065263482740	2.25998487534436
C	-4.56380339817903	2.75123113329536	-0.93932470182641
H	-4.27861928074602	2.67196768935176	-1.98884840047694
H	-5.65246586346107	2.78019934393161	-0.86008656719771
H	-4.15643619979722	3.68284626691997	-0.54246837346293
C	-4.65613072821969	-0.11921028050704	-0.70983474238143
H	-5.74185313297034	-0.02651730807659	-0.66838133720430
H	-4.33922509184526	-0.24528597333320	-1.74483367460542
H	-4.34211495869263	-0.99609672770063	-0.14403630676970

1^Nb ((NH₂)₃P=NH) E = -563.862089817063 au

ZPE = 0.09632658 au

G = 0.06671285 au

P	-4.05916442707731	1.44258132375646	0.03844243954254
N	-2.52748798276287	1.36188281478643	0.23970401446222
H	-1.95697596272281	1.22768739672273	-0.58266868596519
N	-4.69454312464153	1.57313766014660	1.57304256834403
H	-5.68894134934957	1.47169705005311	1.69538319301208
H	-4.14116942528257	1.13967241167563	2.29518943522281
N	-4.91244360713354	2.69749344050702	-0.70047496209176
H	-4.76104307857426	2.77294397410308	-1.69696347699080
H	-4.78298403942315	3.59085243390606	-0.24523869686541
N	-4.68871212060493	0.20225827440044	-0.90221740462072
H	-5.68446062470098	0.15683215817688	-1.06094888142805
H	-4.26160601772626	-0.70142799823456	-0.77279485262177

1^Nc (Tms₃P=NH) E = -1622.013493244690 au

ZPE = 0.35082538 au

G = 0.29950894 au

P	0.10531035714693	0.28716977987980	0.00173669705317
Si	-0.07971409726829	2.55832554711643	-0.28982428911324
Si	-1.55547466154425	-0.39542215209706	1.39721311419776
Si	-0.20790124640059	-0.69454756362702	-2.04699243903034
C	0.64046607797778	3.32165035702410	1.26393038481725
H	0.85090220991573	4.38354055242066	1.11270450314723
H	-0.03843329376633	3.22794440156258	2.11233427192505
H	1.57128390668022	2.81711719851498	1.52990766592732
C	0.98184607812929	3.04076945641959	-1.76704052484007
H	0.57562989400915	2.66322219011600	-2.70674626171244
H	1.04464278577677	4.12960607285001	-1.84588156030662
H	1.99919453849377	2.65837531402464	-1.66065929457478
C	-1.85481740886523	3.12253845928112	-0.56446594877949
H	-1.88002362288640	4.20052031343829	-0.74810276023205
H	-2.31331216115519	2.62971504922454	-1.42319491067400
H	-2.47630551058953	2.92443413969287	0.31054389814183
C	-1.55291402510143	0.14780872073621	-3.05974509067322
H	-1.29770555244566	1.18323435204035	-3.29066022113676
H	-1.69015035580387	-0.37740168082594	-4.00930048008227
H	-2.51219154657320	0.14493560723242	-2.53917362511730
C	1.45608872787087	-0.57579652256590	-2.90911844739828
H	1.44137613535750	-1.13284939143581	-3.84969853832728
H	1.73094381471554	0.45583327819613	-3.13281406392016
H	2.23622732255688	-1.00486874866403	-2.27677981685354
C	-0.62872204234993	-2.50636868812641	-1.78140871503097
H	-1.63386540631423	-2.64165014995921	-1.37883093369859
H	-0.57469493691090	-3.04975282949384	-2.72878402328952
H	0.07997848135604	-2.96512280461082	-1.08949042500732
C	-1.56198680832707	0.75323190131496	2.88008060076957
H	-1.92058842355616	1.75226980873063	2.62742658337372
H	-2.21417914802894	0.35352565694488	3.66150060545229
H	-0.55528094567948	0.84263649138941	3.29152066044240
C	-3.21666274884148	-0.34805914565394	0.51673060337808
H	-3.25721482510105	-1.06246317241530	-0.30736426335934
H	-4.01431441459183	-0.60972968703803	1.21754179017502
H	-3.44124928614292	0.64206204680657	0.11717481715905
C	-1.09474485023396	-2.12958627821323	1.92641579283408
H	-1.69701718884444	-2.44489484826214	2.78261211702263
H	-1.24105012658627	-2.85280178412631	1.12347138825999

H	-0.04100754158855	-2.14688512605935	2.20978755321785
N	1.44408338777511	-0.18872440203242	0.77029036124334
H	2.30105580773568	0.07458679024942	0.29190346462002

1^Pa (Me₃P=PH) E = -801.923709995336 au
 ZPE = 0.12232384 au
 G = 0.08997671 au

P	-3.88152924685475	1.30594492950742	-0.04122780135108
P	-1.82594057710859	0.99280812986256	-0.18903657098662
H	-1.59540559788499	2.26487252002594	0.41471991826341
C	-4.59060125459235	1.51746976332188	1.63315556254296
H	-4.14334347707228	2.39843776523650	2.09464170840180
H	-5.67589368359320	1.63873087282191	1.60174914298912
H	-4.33141866971969	0.64825271846934	2.23623243719067
C	-4.58811082856819	2.72909687809693	-0.94950901636413
H	-4.34047795513741	2.62788970966817	-2.00545537441259
H	-5.67165449373685	2.79356028903279	-0.82540529734045
H	-4.12804360090855	3.64500882561049	-0.57735385150663
C	-4.74196608454506	-0.14537410248814	-0.72250418373611
H	-5.82313963001478	-0.01146932896253	-0.67371477592108
H	-4.44114301356919	-0.28684018574543	-1.76003272696170
H	-4.46056188669399	-1.03050078445788	-0.15297917080759

1^Pb ((NH₂)₃P=PH) E = -850.075506035465 au
 ZPE = 0.09116971 au
 G = 0.06035888 au

P	-4.10904293048280	1.46228628052240	0.08977256125490
P	-2.05511541068429	1.42860906029177	0.36242745537314
H	-1.89382057686062	0.94833325873872	-0.96731490042414
N	-4.77378175268452	1.58820923694854	1.61403681762585
H	-5.76747649023039	1.73189239781909	1.70565306890901
H	-4.35542741146388	1.03794398107887	2.34619084064282
N	-5.03093023218594	2.68866851767327	-0.64174428740500
H	-4.85221385483409	2.75894613069955	-1.63553116868031
H	-4.88090409041299	3.59090776988935	-0.20763815805764
N	-4.64411293477120	0.21840851984242	-0.88964442537882
H	-5.62912030194973	0.14503695793654	-1.09958819952071
H	-4.16758577343931	-0.66363117144061	-0.79616491433910

1^Pc (Tms₃P=PH) E = -1908.263664465046 au

ZPE = 0.34647803 au

G = 0.29447518 au

P	0.07174675943959	0.28390821131164	-0.03044526311844
Si	-0.05951634041166	2.55464857625284	-0.25341608455594
Si	-1.57619372656193	-0.39507142471366	1.38433042144581
Si	-0.23689028653555	-0.69555023691042	-2.07269711294710
C	0.62878808057833	3.31331011653827	1.31013930236511
H	0.83068285386905	4.37626220421597	1.15286328547401
H	-0.06377541902741	3.22025882645870	2.14700839816000
H	1.55906777708902	2.81587905380675	1.58982121932713
C	1.01887161030501	3.00502340650267	-1.72190677687040
H	0.60775168030360	2.63434168457808	-2.66205437027726
H	1.10358152973704	4.09217372742152	-1.80159150994139
H	2.02522761239253	2.59887351329413	-1.60553678312552
C	-1.83135301986114	3.10923027432014	-0.55452727668742
H	-1.85637904143261	4.18899542747485	-0.72733724119101
H	-2.27068246124477	2.62333139630918	-1.42678000427948
H	-2.46856065558656	2.90070452952154	0.30650067890375
C	-1.61068274184408	0.13920618624132	-3.05055634746683
H	-1.36852671535428	1.17913711122271	-3.27609932305958
H	-1.75395346895326	-0.37828626093051	-4.00345100757130
H	-2.56198006654092	0.12070411345488	-2.51664032944350
C	1.39969539684430	-0.55642958533290	-2.96952942287366
H	1.37169579405197	-1.14038682950880	-3.89351003617313
H	1.64318575254286	0.47452268500178	-3.22851809579067
H	2.20033063951459	-0.94697674255825	-2.33884651141342
C	-0.63698304096575	-2.50161512551593	-1.76625024589210
H	-1.63164401661930	-2.64380923865539	-1.34140441549762
H	-0.59557335715081	-3.05541763307856	-2.70804074782163
H	0.09718839121488	-2.93801151270784	-1.08652263267953
C	-1.61142606640772	0.78771446673844	2.83695580329597
H	-1.98467650045124	1.77441447648648	2.55955428305774
H	-2.26931588425700	0.39071995179440	3.61516088457368
H	-0.61361555401214	0.90257520930109	3.26263638432813
C	-3.22796501245726	-0.38352943708337	0.48945254841512
H	-3.25651984854779	-1.11454364717683	-0.32000789753767
H	-4.02674826859855	-0.63805893116765	1.19173596158380
H	-3.45642466339194	0.59685432669940	0.06909693326698
C	-1.13283038113523	-2.11715918381824	1.96511297172910
H	-1.84906136998977	-2.44806415245748	2.72267790738746
H	-1.14328853550874	-2.83961728232471	1.14897841484209
H	-0.13577811707822	-2.12892805716695	2.40789380528034
P	1.89217083577669	-0.37347654927060	0.91551055844001
H	2.68786719626623	0.40027086543121	0.01898991433844

1^oa (Me₃P=O) E = -535.608706204099 au

ZPE = 0.11679156 au

G = 0.08620781 au

P	-3.95361712901369	1.39192245202993	0.00023252286609
C	-4.68917355190878	1.53012369188898	1.65634554126930
H	-4.34673304874425	2.45583548649188	2.12025980733950
H	-5.77979222740546	1.52697138497218	1.61899689730512
H	-4.34727999445241	0.69343003614058	2.26675292390903
C	-4.68791345654820	2.75644593676693	-0.94859012963717
H	-4.34885646889098	2.68963052060339	-1.98307192724331
H	-5.77860611013659	2.72987286877667	-0.92451414280200
H	-4.34075458131145	3.70330615394218	-0.53346315613748
C	-4.68773007020097	-0.11236675111512	-0.70746076002893
H	-5.77843931235434	-0.08219987658616	-0.69049824012595
H	-4.34647728226399	-0.22179662609350	-1.73750297826296
H	-4.34252663353962	-0.97591589277294	-0.13756084402676
O	-2.47043080322923	1.39197469495501	0.00007454557553

1^ob ((NH₂)₃P=O) E = -583.770984400581 au

ZPE = 0.08567916 au

G = 0.05630523 au

P	-4.22916577114712	1.44561587001335	0.03542614981878
N	-5.11335954542851	1.39511430354462	1.45003844509810
H	-5.07567451653798	2.23965567298456	2.00301296707834
H	-4.96606398124779	0.56874604243427	2.01200955704196
N	-4.90997334585715	2.80227586326473	-0.65612968731580
H	-5.90257510416892	2.84392230464881	-0.82539851548485
H	-4.35366622953800	3.25584552037054	-1.36345428097328
N	-4.71451134910129	-0.00426879073565	-0.63376208485683
H	-5.69182456893432	-0.17338209307302	-0.81411965730347
H	-4.10068007321806	-0.37681206552599	-1.34127379337931
O	-2.76115647482069	1.54766730207374	0.01410559027634

1^oc (Tms₃P=O) E = -1641.913553195116 au

ZPE = 0.34032943 au

G = 0.28917831 au

P	0.09880667660085	0.31477121707650	-0.03221312957428
O	1.46600415724303	-0.04565133338614	0.53722226610782
Si	-0.06966356118900	2.57958637541619	-0.32630281340594
Si	-1.56821166947728	-0.36861400513332	1.38003327063654
Si	-0.21041514124284	-0.70025947807537	-2.06197152859488

C	0.68734668725722	3.33187054020601	1.21432613529530
H	0.85144328290949	4.40436637756722	1.08116271102442
H	0.05172008279206	3.19282476856038	2.08975612105897
H	1.64897707208740	2.85781575550823	1.41958975124818
C	0.95687401427666	3.05587076858753	-1.82600518703703
H	0.52085420371172	2.69021514783772	-2.75700028973070
H	1.03498218376846	4.14407104722598	-1.89961812273057
H	1.96769347287786	2.65250053234769	-1.74158341708576
C	-1.85806856992373	3.11960521352028	-0.55407719166323
H	-1.90197790374193	4.19833821061006	-0.72846604987912
H	-2.32793833701163	2.62770438776361	-1.40731406471842
H	-2.45863744036073	2.90638762376441	0.33182655394239
C	-1.59197695982195	0.11778666152441	-3.04278806888121
H	-1.35730620958976	1.15624461984460	-3.28155850270848
H	-1.74079859200196	-0.41202341336150	-3.98787186599478
H	-2.53998555057364	0.10048350160480	-2.50235035804751
C	1.44676434210610	-0.54438104975506	-2.92302165357977
H	1.48553110469495	-1.18165940045376	-3.81032614528608
H	1.65108782611887	0.48141778729835	-3.23181834182448
H	2.24124642451398	-0.85178845068547	-2.24014288029572
C	-0.60059659325982	-2.51704114593597	-1.78153780023650
H	-1.58671593674840	-2.66522095803213	-1.33864587212886
H	-0.57996128485637	-3.05539796250290	-2.73318629372174
H	0.14102240309558	-2.97348318155369	-1.12333418805820
C	-1.60666839805822	0.78833585774868	2.85963183219658
H	-1.97301837549013	1.78199851862727	2.59665653487433
H	-2.26527743761100	0.38591487795335	3.63448431672924
H	-0.60961755982741	0.89601661880696	3.29072964935314
C	-3.24174290987974	-0.38142397719701	0.51857652661299
H	-3.27130127239753	-1.10803812166893	-0.29522413254995
H	-4.02560449448197	-0.65321453483563	1.23121752510498
H	-3.49570381059457	0.59688204632015	0.10717845197502
C	-1.05835437555289	-2.08477766177222	1.93644027854080
H	-1.67284606708772	-2.41967407325503	2.77633825613920
H	-1.15347244922459	-2.81761220646405	1.13437599285688
H	-0.01444547404937	-2.07214673165223	2.25568880403648

1^sa (Me₃P=S) E = -858.202438937130 au

ZPE = 0.11529108 au

G = 0.08379139 au

P	-3.96973404424943	1.39194866810813	0.00028804619673
C	-4.72329490483105	1.52976703926639	1.65365150994852
H	-4.38468531250633	2.45536570346497	2.11848825140849

H	-5.81359887998296	1.52471978657609	1.59655074236693
H	-4.38473033453774	0.69369853716562	2.26512193422808
C	-4.72236149385344	2.75420472003390	-0.94692888291318
H	-4.38754769354577	2.68815339048380	-1.98189263222752
H	-5.81275136951796	2.71147481913796	-0.91085669794036
H	-4.37858555906527	3.70188911021657	-0.53325674490460
C	-4.72191554563626	-0.10979055433742	-0.70639695284154
H	-5.81235472894970	-0.06085891431025	-0.68226150131976
H	-4.38312421104115	-0.22091933911206	-1.73612266160003
H	-4.38160884812518	-0.97418855060077	-0.13659671679218
S	-2.02203774415773	1.39176966390708	0.00021236639044

1^sb ((NH₂)₃P=S) E = -906.355098465257 au
ZPE = 0.08362675 au
G = 0.05323983 au

P	-4.26071343493483	1.44355981097919	0.03188107871868
N	-5.17933301564245	1.39064078038231	1.43699792536307
H	-5.11355814603364	2.23300680098468	1.99276534625568
H	-5.00532557581342	0.56926777931844	2.00072977158169
N	-4.94973234913506	2.79832413440861	-0.65822713225702
H	-5.94620740981162	2.82752278011764	-0.81559526250810
H	-4.39919305237377	3.26752187965086	-1.35903094083580
N	-4.75434119982502	-0.00629906160847	-0.63493651001349
H	-5.73720240936550	-0.16256792795014	-0.80476260301368
H	-4.14425945148979	-0.39473645565159	-1.33630850187739
S	-2.32878491557475	1.57813940936843	0.02694151858634

1^sc (Tms₃P=S) E = -1964.532356591744 au
ZPE = 0.33917249 au
G = 0.28765550 au

P	0.06302160847838	0.32352238922734	-0.04671795853112
S	1.86309958491303	-0.16429081088329	0.71708240299944
Si	-0.07502349416567	2.58952808163802	-0.31630789786775
Si	-1.58210400979795	-0.37878027466147	1.37480862356724
Si	-0.20934140476541	-0.69268075364707	-2.07650570634439
C	0.63506997566145	3.36106542538788	1.23146536051615
H	0.79130634236544	4.43223320844709	1.07815608963246
H	-0.02268206359508	3.23449999381736	2.09181462126980
H	1.59472935466812	2.89899428100812	1.46850023393918
C	0.98482252008543	3.02690532212971	-1.79964311113968
H	0.55145878756891	2.67194026011127	-2.73583350553591

H	1.09430369546117	4.11224763821643	-1.87289812789897
H	1.98096634953446	2.59360846402886	-1.69465813132372
C	-1.85965119579197	3.11831016809050	-0.58563374442033
H	-1.90180082258014	4.19486701996802	-0.77352432476809
H	-2.31369712646770	2.61470440016346	-1.44022310045370
H	-2.47414199798618	2.91558397560211	0.29319464356506
C	-1.62395490666169	0.09734781388202	-3.03035408388851
H	-1.40896097991392	1.13772971731660	-3.27959133338134
H	-1.77998963299855	-0.44018328037981	-3.96992288887760
H	-2.56122175962873	0.06819450865714	-2.47265150167417
C	1.41558299543157	-0.50900962455951	-2.98215717103660
H	1.42499642465781	-1.14819671960413	-3.86915322905435
H	1.59553069728482	0.51783862751065	-3.30112138283899
H	2.23652647184179	-0.80712894342577	-2.32785035511295
C	-0.55853287512045	-2.50559607529677	-1.74878739188917
H	-1.54826150032250	-2.66662290468254	-1.31914066224076
H	-0.50685396206582	-3.06786180217679	-2.68507842194404
H	0.18572945950619	-2.91933606315538	-1.06620717893526
C	-1.56562693150467	0.78165309064169	2.84682376619264
H	-1.93716502930520	1.77594890551196	2.59470335058074
H	-2.19986454008269	0.38131755793774	3.64251236190174
H	-0.55283967550283	0.88128600151156	3.24097460248323
C	-3.25784735219186	-0.35227205023025	0.52113760390281
H	-3.30185166700609	-1.07139573224528	-0.29873412736220
H	-4.04104294143722	-0.62057122888636	1.23585164721660
H	-3.49924434715964	0.63335179491809	0.12059118158267
C	-1.11544090652172	-2.10764434225683	1.91260870045569
H	-1.74247754754399	-2.42233721852912	2.75125192204400
H	-1.23551384649105	-2.83424895771433	1.10877450365825
H	-0.07196419084979	-2.12592109338895	2.23132080101193

2a (SiF₄) E = -688.311382894961 au

ZPE = 0.01250444 au

G = -0.01617953 au

Si	1.12779234297591	0.37734539763511	1.97439471198149
F	1.02191724372951	1.92653502082133	2.18740645747247
F	2.24468589890300	-0.20332214190157	2.90864988346270
F	-0.24777417911370	-0.28987271035102	2.32163517946315
F	1.49388249453148	0.07872288463864	0.47973037790828

2b (Si(CF₃)₄) E = -1638.090475910649 au

ZPE = 0.05659171 au

G = 0.01248369 au

Si	-1.06326064765221	2.96024429454895	1.25846931968960
C	-2.99800423096455	2.96561526590767	1.25891265635524
F	-3.48265832421734	2.33563583872770	2.34664541358038
F	-3.48571376529149	4.22075895948440	1.26047044660810
F	-3.48354213793558	2.33796181195985	0.17024974089833
C	-0.41135384256008	3.86456087973650	-0.32393790452606
F	-0.80952100643306	3.23507674780107	-1.44627511474271
F	0.93495429115284	3.90897937433060	-0.33503347189116
F	-0.86508044623080	5.13136481059733	-0.38219966498246
C	-0.42082006330249	1.13552851805707	1.25890007405413
F	-0.84797471445787	0.46778705194709	2.34802726765252
F	-0.84983441041862	0.46630954768102	0.17142794395355
F	0.92604276085071	1.09881274982566	1.25778333091618
C	-0.41167983858176	3.86438572469016	2.84103875701461
F	-0.86248638528737	5.13230640641014	2.89735258964172
F	-0.81338454153284	3.23685557721948	3.96321321316690
F	0.93469163286252	3.90560363107530	2.85453678261112

3^ca E = -1187.964940156954 au

ZPE = 0.15427384 au

G = 0.11560088 au

C	-1.88817585208840	0.40221925994948	1.07392778032346
H	-2.25150886467896	1.42967790344408	1.02672715063788
H	-2.27749722365936	-0.09558527463934	1.96319645219227
Si	0.06545088169143	0.36316828608947	1.10073488548006
P	-2.49953641460911	-0.45548229422509	-0.34185566343423
C	-1.92413300684287	-2.16046453259579	-0.37037315193691
H	-2.35659035596812	-2.68350435259879	-1.22403071432442
H	-0.83690206425368	-2.16344251495706	-0.43065907958974
H	-2.21510349717068	-2.65750952258824	0.55453302005436
C	-4.31011511008631	-0.50124054387759	-0.36683536414071
H	-4.70217132613180	0.51605851669374	-0.37452408001399
H	-4.67165168474125	-1.03202735168405	-1.24835780305070
H	-4.67043770718342	-1.00847528702606	0.52861691621808
C	-1.95932223037707	0.35882541078366	-1.85444837718898
H	-2.35660494585219	-0.16608122958299	-2.72385023214007
H	-2.30959521602891	1.39092107102247	-1.85803404545175
H	-0.87008508208530	0.36175917156676	-1.88069321030843
F	0.05252820302927	1.83600205584234	0.30367992228433
F	0.91024950193397	0.96518366810066	2.33081739388511
F	-0.04758554620854	-1.13922791868445	1.84449211185083
F	0.79045181131136	-0.33890405103317	-0.18939661134643

3^cb E = -2137.770306927036 au

ZPE = 0.19962280 au

G = 0.14792225 au

C	-2.49612503579728	-0.52710479245635	1.06743204367996
H	-2.87358866652797	0.49713323729719	1.09204633090459
H	-2.83158005778002	-1.02152504569380	1.98150913209932
Si	-3.39469199276341	-1.42108882860398	-0.42281306579036
P	-0.73229760199961	-0.37598233857652	1.24659613080638
C	-0.42871619182977	0.55042204182470	2.77130468839274
H	0.64207481657126	0.67534568875335	2.93484988213646
H	-0.897531107257201	0.53220211550006	2.70166107661701
H	-0.86043834257680	0.01382335001981	3.61659825490420
C	0.06194305412683	0.53880576954420	-0.08114905300112
H	-0.01571667023511	-0.01661778521317	-1.01228132021544
H	-0.42221618806034	1.50517607720965	-0.21190453303780
H	1.11114662900006	0.68409786050520	0.17972335446665
C	0.11228248684177	-1.95300412032951	1.42111337316873
H	1.15564565704088	-1.76211619086113	1.67591119448151
H	-0.35621128733535	-2.54423547158176	2.20615630357216
H	0.05305035145220	-2.50875436276156	0.48857629926546
C	-5.37718558138693	-1.43894480452085	-0.39311583432353
C	-3.41357045542315	0.35087283509841	-1.46326867644326
C	-2.38042368368477	-2.27398394845209	-1.91361790523320
C	-3.33944901640023	-3.19229836286768	0.61449571045138
F	-3.67898640861779	-3.04785405142659	1.94171044680268
F	-4.12360137130645	-4.18059606777932	0.14398910849150
F	-2.06412637259635	-3.71965900109136	0.66447275426368
F	-5.91299037720008	-2.10163697311904	0.65736190003569
F	-5.93296662675736	-0.20451228062248	-0.36571576949645
F	-5.83573474516834	-2.05081370961054	-1.51582674532786
F	-4.23824174078631	0.40236017865424	-2.52643465392987
F	-3.74937484365768	1.43448500669234	-0.68232591622580
F	-2.16113937073174	0.67790652983874	-1.94389891022800
F	-2.59722140574073	-1.74414740049142	-3.12914834903387
F	-1.02128793524462	-2.11095689886158	-1.67011264169051
F	-2.56906519816736	-3.59778247601702	-2.04314748056303

3^cc E = -1236.125801984793 au

ZPE = 0.12348659 au

G = 0.08649081 au

C	-2.49917602968998	-0.35700854079321	1.34225227653799
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H	-2.83047532920835	0.67985885300702	1.33377918742509
H	-2.84393893865021	-0.86965918753062	2.23852613435120
Si	-3.13581136655371	-1.28302887577139	-0.26116651463963
P	-0.74523106120538	-0.39375505949573	1.30739742933220
F	-3.03679938140320	0.19982948500034	-1.06692915948558
F	-2.02968675581508	-1.89580305956157	-1.29044461836425
F	-4.70348798279079	-1.43219696794724	-0.55874919827979
F	-3.07694498575819	-2.71836086334593	0.62824320589508
N	0.20052712008947	0.28708987250120	2.48108612606554
H	0.22400414985416	-0.16137008183103	3.38390627157338
H	0.24408573746520	1.29385864500009	2.51956010429825
N	-0.33114680730758	0.49934691287777	-0.00364152990537
H	-1.01211113929769	0.52204781277613	-0.75842194074205
H	0.63205287561727	0.55337813450018	-0.29495435903575
N	-0.35668005495237	-1.98027086598996	1.45146002939002
H	0.60356353644634	-2.27458368351284	1.36833244447538
H	-1.04277583683984	-2.64112443988314	1.09656233110822

3^cd E = -2185.926637413158 au
 ZPE = 0.16755731 au
 G = 0.11669995 au

P	-3.21035600788576	-0.37628316547673	-0.43708153666623
Si	-0.49642424756185	0.51151207981386	1.09460984129199
N	-4.79743268357869	0.06342299155071	-0.37324084244269
H	-5.40219404107666	-0.19804505624577	-1.13810191316282
H	-5.25801205465827	0.06552531301280	0.52422870095156
N	-2.81309505558181	0.12089801131822	-1.95000119784000
H	-1.87261237057418	-0.12251423965389	-2.23761748773501
H	-3.01887596064599	1.08651528885675	-2.17068135837692
N	-2.90556011699033	-1.97460014026295	-0.37145330482789
H	-2.18672118056098	-2.32015006919075	0.25342153794807
H	-3.10368893571252	-2.56098923470191	-1.16638590200911
C	-0.43381706976440	-1.23454842831096	2.19248641815309
C	0.75394930208716	-0.29165476129953	-0.23933444234497
C	0.18597666776813	1.54803183151795	2.63571317417786
C	-0.55508698040699	2.23092824813991	-0.04781197688175
F	-1.62211865094185	3.04498691155006	0.25419292881697
F	0.53471419601762	3.01845044462323	0.02996908711308
F	-0.72386424360809	1.96804625305172	-1.39457642099699
F	-0.34967875239296	2.79019881867871	2.71402450480675
F	-0.04545567400387	0.97448658448530	3.83747238578602
F	1.52942989173801	1.70333836757603	2.53157377600303
F	0.72127823165899	-1.51885399575430	2.81396578682188
F	-1.40614873697136	-1.30433806974802	3.15527990988037

F	-0.70029438367021	-2.35484350302727	1.39324578449946
F	0.01862826287112	-0.86364718142706	-1.27091462233458
F	1.53622025855857	-1.27729317340959	0.23054726362788
F	1.57769136339404	0.59531999149837	-0.82283294086005
C	-2.43878692687433	0.35748903953926	0.97519005720913
H	-2.82847670508801	1.37419549544376	1.03064647430591
H	-2.79288592554434	-0.19096271214797	1.85001323508595

3^ce E = -2294.303688982847 au

 ZPE = 0.37867202 au

 G = 0.32208281 au

P	-2.56138351335546	-0.48299205981433	-0.43756189218492
Si	-0.24777443026130	0.54571721983160	1.54066518296111
Si	-4.85277392452691	-0.51797896836861	-0.35688076023101
Si	-1.74031274599323	-2.63716123766060	-0.28048150818294
Si	-1.84126408702853	0.78575795862520	-2.23564068375397
F	-0.65290539482019	0.80569128434971	3.13177958206312
F	0.59707747862929	-0.79404737264716	1.91544048986503
F	0.47012351486554	1.99302291492335	1.42619102614277
F	0.13080586957938	0.27240374219000	-0.11755435331928
C	-5.33391700868573	-1.46346528722685	1.18837744535564
H	-4.84716154977874	-1.07094582388441	2.08181998571465
H	-6.41427846279446	-1.37972294647706	1.33607704716276
H	-5.09435627501115	-2.52458468591643	1.10675427354767
C	-5.38994586254995	1.27279059597863	-0.21147549289701
H	-5.08397875638410	1.86942681390813	-1.07175938472835
H	-6.48066113227124	1.31950700442504	-0.14878788318227
H	-4.98608167048823	1.74139017226659	0.68710443861622
C	-5.63708840691851	-1.32700219716480	-1.85389191012517
H	-6.71748464327308	-1.37799271653653	-1.69008986489175
H	-5.46914443993250	-0.76298176359456	-2.76999196082868
H	-5.28096814803492	-2.34476122311091	-2.00929753381349
C	-1.88798681562154	-3.07690115987995	1.53002879566492
H	-1.61323075251166	-4.12821103727872	1.65654042994968
H	-1.20089049459321	-2.48047175998139	2.13100902974571
H	-2.89800785939036	-2.94914892868856	1.91922035029591
C	0.02387262249137	-2.75242033042999	-0.86060471261689
H	0.12081593820499	-2.57807097732393	-1.93161622592765
H	0.65467784929767	-2.04163082118981	-0.33038288887041
H	0.38147906287434	-3.76508243652913	-0.64973505479822
C	-2.85248752617744	-3.71787137105634	-1.34085031034207
H	-3.86462998639079	-3.79534397960313	-0.94261638281390
H	-2.91456484443973	-3.36169140761694	-2.37106126263859
H	-2.43316800985036	-4.72741050641837	-1.36936680640453

C	-0.33730257885409	0.05478324644411	-3.06068528431389
H	-0.05141461622755	0.71229370322684	-3.88742782126979
H	0.49749011563422	-0.02221295915346	-2.36906922573830
H	-0.54853722043172	-0.92811516610707	-3.48575021329632
C	-3.23161123770531	0.78837809733987	-3.50405054668698
H	-4.15353342506192	1.23840034741876	-3.13570250941261
H	-2.90162190960961	1.38054518477137	-4.36283780229035
H	-3.45957063911922	-0.21379426734645	-3.87147840785941
C	-1.58776759822604	2.51466575873299	-1.57840148801010
H	-0.76805711381699	2.55638464780411	-0.86244926159875
H	-1.34582474469260	3.17400242745928	-2.41731671033823
H	-2.48989256946871	2.90711042022359	-1.10475665016892
C	-2.11387688234430	0.37641399121503	1.11765505380781
H	-2.51804148839302	1.39060073379586	1.07059863356047
H	-2.62116445654164	-0.11964101392441	1.94423191908139

3^f E = -3244.107317559104 au
 ZPE = 0.42423690 au
 G = 0.35517925 au

P	-2.38577402179485	-0.61706289943807	-0.46833759980555
Si	0.07372159348838	0.78395853222876	1.50815677819562
Si	-4.58834479466900	0.00285154947814	-0.18273409497461
Si	-2.29291312619350	-2.93824932821939	-0.51709430852078
Si	-1.68180635068478	0.15417268402123	-2.53388686987007
C	-5.22131701784438	-0.98450811419273	1.27859580229998
H	-4.58660467751197	-0.85302449841900	2.15641034949561
H	-6.22170873863532	-0.63015262335296	1.54212420984784
H	-5.29454446610480	-2.05126233361889	1.06673017335629
C	-4.59954830348872	1.83074933402523	0.20228508901177
H	-4.11008713705055	2.42256227653395	-0.57018123318828
H	-5.64229660143196	2.15593492415786	0.26759419354064
H	-4.11883401727173	2.06947643192044	1.15024928820867
C	-5.59488059721686	-0.33624301175976	-1.72548057330038
H	-6.63922895347709	-0.09088356499740	-1.51187097536075
H	-5.28007595481724	0.28930026759427	-2.56148537709787
H	-5.55948105593697	-1.37773454606725	-2.04073482176836
C	-2.28431782867460	-3.52770801245645	1.25319488717558
H	-3.12376034883314	-3.13330939916884	1.82728742609783
H	-2.37513217605761	-4.61808440583094	1.24416949582992
H	-1.36107415702208	-3.27431092128985	1.77083406659584
C	-0.80097224865105	-3.54657549262746	-1.46404478117423
H	-0.80370234717183	-3.23302867764639	-2.50723285577577
H	0.13363276927698	-3.23142393221017	-1.00712517617679
H	-0.82759210060776	-4.64069639210033	-1.45327568474853

C	-3.85191968375615	-3.54189380137074	-1.37171305404602
H	-4.75804433319785	-3.28125457902465	-0.82546318132552
H	-3.94764906437479	-3.17967186549278	-2.39444818012121
H	-3.80239951026970	-4.63394087088089	-1.41595543120929
C	0.16915208767531	0.02825511682468	-2.66310534666023
H	0.43547727903007	0.00761336131523	-3.72411799889203
H	0.66364738749449	0.88580789591640	-2.21396585636814
H	0.56742747028831	-0.87385849493969	-2.19999273860500
C	-2.51456278870703	-1.03218090359418	-3.73174736138357
H	-3.59914722872871	-1.04463432080324	-3.63004796008757
H	-2.28869969554633	-0.67983686636514	-4.74261976708370
H	-2.14908009209194	-2.05445644606974	-3.65704135081752
C	-2.32937460669688	1.86684518305898	-2.89870801133273
H	-2.06238388512041	2.10314671391766	-3.93354926408881
H	-3.41631307146325	1.91921696018883	-2.82492621522969
H	-1.89719587780169	2.62821332514982	-2.25528210274013
C	0.17740768670439	1.17969278383787	3.44436575159837
C	-0.74658657196051	2.61744534257109	1.13706540068938
C	0.85230066957632	-1.07779826070184	1.78140621262575
C	1.67780650521340	1.28217741543204	0.42513131898535
F	0.04139857485148	3.70554280082303	1.19928639998764
F	-1.81753722666515	2.89173235565953	1.95214420985369
F	-1.29512607504042	2.62911329033441	-0.14101129989250
F	-1.01303800609167	0.84809126701304	4.03732275696605
F	0.38981385723097	2.48321920974520	3.72755552454452
F	1.13138251035901	0.49232655164458	4.10839298740346
F	0.18379805501132	-1.78750554136980	2.74988115552577
F	0.65793687168241	-1.83210419921240	0.62855121949619
F	2.15764662570886	-1.20470385255111	2.07757917958463
F	1.45611027966279	2.21190838730322	-0.54331537281503
F	2.60054517850299	1.81996401096823	1.26266093721585
F	2.29194983508424	0.25323934490025	-0.21039987218174
C	-1.65774640755644	-0.02149998775851	1.11903884107344
H	-2.36624510485988	0.71222467511727	1.49750033364606
H	-1.72964833576401	-0.87949388815047	1.78618846779079

3^{Si}a

E = au

ZPE = 0.14397456 au

G = 0.10332560 au

Si	-1.92959967927340	0.61342040154887	1.52135965847564
H	-2.65505210113484	1.89722157370337	1.32389333580532
H	-2.68717795958802	-0.17812307130883	2.52796196166288
Si	0.42493013028651	0.35718889661480	1.12197913469499
P	-2.62126866949911	-0.47287802580048	-0.37438582385786

C	-1.96787299582472	-2.16251422327940	-0.39884816546767
H	-2.28611179859126	-2.67721578730937	-1.30635629986221
H	-0.88045465823510	-2.11826129849348	-0.35634351120505
H	-2.33094968692648	-2.70457366661682	0.47432207295036
C	-4.42351370310266	-0.61250966779761	-0.57929367542310
H	-4.86826234076538	0.38185562432528	-0.60978535403018
H	-4.66083076909430	-1.14209962268993	-1.50371742846886
H	-4.84467936063827	-1.15797323697252	0.26498473668376
C	-1.99340545148444	0.37822215750465	-1.84566000231459
H	-2.27586392096145	-0.16755179015414	-2.74689161128045
H	-2.40670653977556	1.38603467308558	-1.88432876946636
H	-0.90882761984580	0.44971121613552	-1.77549358851887
F	0.23796775677304	1.76263381392424	0.22930903242421
F	1.67491892777844	0.91715171805152	1.95447670074519
F	0.27496295939096	-1.02772964659970	2.04240214120110
F	0.79946175051184	-0.50013956787150	-0.21591724474822

3^{Si}b E = -2388.779364013978 au

 ZPE = 0.18933028 au

 G = 0.13600848 au

Si	-2.77220039095898	-0.31799605897472	1.41860578532804
H	-2.99530043081991	1.14097474534212	1.54712496333401
H	-2.93055199314074	-0.92674655691923	2.75953225741626
Si	-3.67953481137688	-1.49245603565166	-0.50723549858953
P	-0.47514379048096	-0.30903951563219	1.33424482123603
C	0.16372988584623	0.28988896099322	2.92793019859382
H	1.25437728967584	0.31946853277739	2.91103734378472
H	-0.22015951963456	1.29109828710759	3.12291214467301
H	-0.16742964238664	-0.37384817327121	3.72611953248669
C	0.20880981453985	0.78646757376666	0.06548018144680
H	-0.06484914090535	0.41646017318263	-0.91969483196214
H	-0.20105641586915	1.78847718373376	0.18369828342578
H	1.29483709983572	0.81885462607663	0.16463142283742
C	0.25417671997635	-1.94500336183120	1.07331765758358
H	1.34135761072710	-1.86445437730321	1.12043672317943
H	-0.09934695234620	-2.63473135539812	1.83741359597897
H	-0.04014777448072	-2.33115494976106	0.09952630737455
C	-5.60629808715680	-1.68070602065557	-0.92955810564645
C	-3.60730384831074	0.30209924373685	-1.47945117906080
C	-2.37514598930646	-2.28507467952278	-1.77598628589616
C	-3.71179261551736	-3.14469973720779	0.67852683350598
F	-4.64653661684215	-3.01332028279779	1.66332726365262
F	-3.91533570375449	-4.34894743834612	0.11720654912922
F	-2.50426016938246	-3.25675464897417	1.36053140257259

F	-6.36278301904076	-1.01159550614616	-0.01582413955674
F	-5.93194984121636	-1.18144229259390	-2.14216697672979
F	-6.03889407434886	-2.95946166055920	-0.91991580504084
F	-3.64600605655698	0.30006897974494	-2.82505239155917
F	-4.59836289767170	1.13311259486226	-1.05804500634816
F	-2.43629223639586	0.98113020842319	-1.15483440416630
F	-2.94049251160783	-2.55057073712372	-2.96935884579381
F	-1.32441232642279	-1.43569891076060	-2.02498027297575
F	-1.79403684466904	-3.43538303031672	-1.35875239421390

3^{Si}c E = -1487.116714117082 au
 ZPE = 0.11257774 au
 G = 0.07456433 au

Si	-2.91066306636197	-0.18704671914504	1.52373955901536
H	-3.06752447813913	1.28381922139746	1.63750029581695
H	-3.14249840299139	-0.79899777823459	2.85522696683072
Si	-3.29340612913164	-1.39242933337110	-0.51232481540426
P	-0.63498810671873	-0.36682107374529	1.37490141430658
F	-3.46797255792518	0.10690120795120	-1.22432022277471
F	-1.97570820410955	-1.71580223721099	-1.41549299428892
F	-4.68248888019543	-1.97280695319579	-1.05510936161721
F	-2.97566211787669	-2.75100663444501	0.45574445038981
N	0.47927424126827	0.24218522160373	2.45997955055961
H	0.49155471537472	-0.19981427848566	3.36791249057304
H	0.53627503242616	1.24889708590863	2.51753678557114
N	-0.21646170996490	0.48982178779226	0.02330506384672
H	-0.85326120734897	0.43059891696164	-0.76261538690365
H	0.75470853065422	0.50871223622607	-0.25632748350686
N	-0.33081644411345	-1.98161129686302	1.47612979982870
H	0.60887391370458	-2.32537409238449	1.33947443561101
H	-1.05926737855084	-2.59097719076000	1.11153767214590

3^{Si}d E = -2436.927588689485 au
 ZPE = 0.15708124 au
 G = 0.10483331 au

P	-3.35140643233820	-0.54371157609808	-0.66987251326297
Si	-0.34615732462962	0.63323935609721	1.26942869499612
N	-5.00488098188537	-0.55948549910067	-0.75100095242843
H	-5.45161500868234	-0.95298870383269	-1.56845848092977
H	-5.52103610865369	-0.70819255357211	0.10270568812317
N	-2.99026362417365	0.12358983653447	-2.14425382517471
H	-1.99635801714378	0.20924004204558	-2.32293862121798

H	-3.46841756711628	0.99018688947022	-2.35276196464398
N	-2.57316105761472	-1.98011078125098	-0.70918256526188
H	-2.02767651140763	-2.29210644516761	0.08127995793881
H	-2.44078036317785	-2.48588570464777	-1.57089773205411
C	-0.36200949711820	-1.07912088925732	2.39143835833876
C	0.59872105041068	-0.25108866903298	-0.23737067957880
C	0.74562018085464	1.55702910380761	2.64326844074834
C	-0.52484613427655	2.36152588839962	0.19616338398955
F	-0.94533929430099	3.38612153036334	0.98583419374039
F	0.55563662982891	2.80278798379008	-0.47607766356221
F	-1.52427748216360	2.24387203134308	-0.76657012351918
F	1.47535466536921	2.58036031073319	2.15190031457536
F	-0.05109069324571	2.08028559438115	3.61577266057465
F	1.62078553110694	0.73444226320026	3.26296739864644
F	0.77491744478601	-1.78102188570732	2.52625894816781
F	-0.82063870599820	-0.83281811198632	3.64674534721152
F	-1.28897753515833	-1.99970307606960	1.87344786743808
F	0.08115572323972	0.09233304391013	-1.46306717078630
F	0.57127347716065	-1.60499719888884	-0.21834147985196
F	1.89733330548677	0.10844244958510	-0.26576479351167
Si	-2.76620697865937	0.53847645256310	1.27240116057639
H	-3.52249363511267	1.79809065743532	1.11040209760119
H	-3.44686358538656	-0.30417039904723	2.28309097311731

3^{Si}e E = -2545.322688972603 au

ZPE = 0.36944153 au

G = 0.31165744 au

P	-2.64089256990149	-0.47710946160411	-0.43566136498352
Si	0.37311873787246	0.56781917817197	1.55932700932485
Si	-4.93493889057165	-0.46011252755808	-0.38597619943456
Si	-1.90518227602958	-2.66699927232486	-0.29614776412444
Si	-1.85245532175651	0.74381085597976	-2.23554885430531
F	0.24715843293283	-0.64770020018976	2.70468829350916
F	1.16560051253131	-0.41139557161147	0.52713995669302
F	1.30736841573431	1.49339582834913	2.48651150476362
F	0.23129575951577	1.76182845880555	0.36329188775025
C	-5.43919728927139	-1.38956336687102	1.15892802384412
H	-5.00317314409901	-0.95007641760560	2.05602911129186
H	-6.52758495505664	-1.35390328649458	1.25925285783984
H	-5.14591104663860	-2.43951163106378	1.11856807143306
C	-5.47837489762497	1.32846320339524	-0.30187931533097
H	-5.24709454384080	1.86542235943082	-1.22300207926430
H	-6.56248493901648	1.36511181529892	-0.16279446279054
H	-5.01241093022330	1.86019822489233	0.52787874236513

C	-5.68300641865231	-1.27446751259496	-1.89817972119432
H	-6.77213693454304	-1.24254871695893	-1.79765233813043
H	-5.42252319522358	-0.75656024680608	-2.82017641056844
H	-5.39208561520957	-2.31843648485806	-1.99985281908299
C	-1.82857639301384	-3.07492563619205	1.52181920798169
H	-1.56091806126004	-4.13045336581823	1.62918866828866
H	-1.07153307863421	-2.48064575955681	2.03633498876163
H	-2.78566531915009	-2.92136218919033	2.02166313550696
C	-0.24547816689015	-2.84526396656852	-1.12203457305605
H	-0.31507435083741	-2.72119036774118	-2.20318283931401
H	0.48890988498770	-2.14550723379485	-0.72712721561042
H	0.11438009015316	-3.86054847074706	-0.92837751812354
C	-3.15236334161569	-3.75645601512647	-1.17998620280014
H	-4.12857986395153	-3.76696630374407	-0.69523329173166
H	-3.28683390748229	-3.46597906428965	-2.22324751230688
H	-2.77196745573694	-4.78213766458169	-1.17174182763591
C	-0.06775985469395	0.33313560164646	-2.57201546466932
H	0.30493496213575	1.06849090419783	-3.29221003856436
H	0.54587485857684	0.40187448202336	-1.67594886629504
H	0.05270320242788	-0.65468277153286	-3.01519915308264
C	-2.90869758810122	0.28291447003095	-3.71814726124826
H	-3.92782550538006	0.66160091177556	-3.63472402426567
H	-2.46444480621797	0.73255486189209	-4.61104982783443
H	-2.95377600069068	-0.79532249841458	-3.88111959397541
C	-2.07811711268159	2.54217537063410	-1.79127791046831
H	-1.40272539737008	2.81742484309702	-0.98155298893372
H	-1.82741669444883	3.15007082382215	-2.66589556324584
H	-3.09984656511306	2.78314935035523	-1.49831657709369
Si	-2.00115582544623	0.60838962882031	1.50771237989613
H	-2.67979161724504	1.91632050713607	1.31795616912112
H	-2.80166575324782	-0.13669381591512	2.51289046109409

3^{sf} E = -3495.133782579800 au

 ZPE = 0.41449044 au

 G = 0.34438995 au

P	-2.66630450634824	-0.61112772830700	-0.53542965857468
Si	0.56646569998184	0.87231656588509	1.67814574288169
Si	-4.94144616636234	-0.27980528760536	-0.31478596990824
Si	-2.28688451706107	-2.89058707898960	-0.53358432889171
Si	-1.99217598699705	0.29013346973916	-2.54973708336048
C	-5.55324780134919	-1.44573622285245	1.01515650720250
H	-4.99218970225941	-1.32986339931456	1.94337246305159
H	-6.60082930289849	-1.21511561172233	1.22858172800381
H	-5.50119397973268	-2.49103148206903	0.71141931191878

C	-5.25984709845555	1.49401268540994	0.17951599246756
H	-4.75981133479022	2.20899345573291	-0.47328175649536
H	-6.33664009486255	1.67812968120231	0.11676226162746
H	-4.94409241275536	1.69576044363911	1.20239713637397
C	-5.78537601384446	-0.63828273374133	-1.94883658146096
H	-6.86635830233866	-0.56583756763050	-1.79703309966300
H	-5.51522292224186	0.08866631940211	-2.71537916006375
H	-5.57107182237049	-1.63619548625193	-2.32924121811097
C	-2.49268729558498	-3.53913745614346	1.20372707397549
H	-3.50767774078089	-3.39316770733065	1.57217468810524
H	-2.29861977991171	-4.61597842972761	1.18681414218437
H	-1.79660705977353	-3.08570798542867	1.90475989597893
C	-0.59087316954494	-3.18858674492192	-1.25332507905159
H	-0.55936242567108	-2.94293640941492	-2.31590137791488
H	0.18507302825149	-2.62681833085604	-0.73762810046723
H	-0.35252878818095	-4.25157030814886	-1.15406061005471
C	-3.59267545410160	-3.66288717080429	-1.64027613264435
H	-4.59908584552638	-3.55621973754661	-1.23527409700271
H	-3.58453788304424	-3.26181674215233	-2.65296928445485
H	-3.38274389934915	-4.73449015377423	-1.70971525427749
C	-0.13520962066210	0.33437641440260	-2.61789725009596
H	0.16294777691306	0.52519163365666	-3.65341804316534
H	0.27193652206579	1.13253804094878	-2.00327932035303
H	0.32554513216543	-0.60290209552944	-2.30967247958079
C	-2.65317118267478	-0.83022317508955	-3.90161223393855
H	-3.72834883293919	-0.99218406651417	-3.84825223134108
H	-2.43651648384735	-0.35953409635388	-4.86521078451134
H	-2.15611507480744	-1.80103803717437	-3.89853086296970
C	-2.74615793413474	1.99670264414546	-2.66117697340498
H	-2.38304597354652	2.48318589501499	-3.57096135269359
H	-3.83511987712597	1.96841928066998	-2.71493943067126
H	-2.44947198881937	2.61823583757666	-1.81589928131518
C	0.99946470163641	1.61378570298254	3.46444020167585
C	0.25770651799050	2.74288033702678	0.92175779588900
C	0.71610923051801	-1.03504949685672	2.39046372485892
C	2.07517830359359	0.51763411494145	0.42966349334157
F	1.32774245788843	3.53554368523964	0.71940385600340
F	-0.60379319943228	3.46268735932248	1.69630856719842
F	-0.37782996521629	2.65889865385854	-0.31336198517664
F	-0.14360989350529	1.74613963816379	4.20197920758672
F	1.57082590042869	2.83735682918245	3.42740773382340
F	1.83043860555524	0.83232953153950	4.18849917522789
F	-0.00932334555126	-1.22027070043297	3.53067372054429
F	0.13837968931714	-1.91436144427014	1.47986514756635
F	1.94053712435088	-1.53979079246373	2.63421066496602

F	2.19008712649398	1.37427721869095	-0.61155186215864
F	3.250591744408506	0.57685341282936	1.09979253858570
F	2.01383905333645	-0.72361598624928	-0.13383188496147
Si	-1.80548139526764	0.45579039064766	1.32669351110001
H	-2.58924864354189	1.70620961396527	1.27013630683329
H	-2.41587324736184	-0.39948923014812	2.37273991976247

3^{Na} E = -1204.046468975972 au
 ZPE = 0.14368853 au
 G = 0.10517019 au

P	-0.78260861545272	-0.29652270458448	1.12458018957204
Si	-3.42286688315109	-0.81575759355681	-0.34369949325324
C	-0.58328052435014	1.43770870312255	0.68200486349654
H	-1.19779811573680	2.04415660706533	1.34786825179338
H	0.46197378333527	1.73564512836681	0.77644208863518
H	-0.92288158233290	1.57543917026924	-0.34213438062098
C	-0.22524757337894	-0.46831398835905	2.83466552344466
H	0.80955861560122	-0.14012115085729	2.93170188899935
H	-0.85198698225630	0.13834685281697	3.48898993983277
H	-0.29576242238620	-1.51227098704834	3.14146141509131
C	0.33654968153652	-1.27833877267965	0.11194869887013
H	0.27314011022331	-2.32059953872104	0.42546250911978
H	0.02673928674533	-1.19785563658806	-0.92731162331124
H	1.36130405275997	-0.92317022257579	0.23028542280891
F	-4.59777853437984	-1.36111807735496	0.68865059448207
F	-4.24331032565228	0.51066653931729	-0.74469542008499
F	-2.05887415486502	-0.26160820116285	-1.21350152393589
F	-3.53413292688637	-2.09938756435308	-1.30646871053516
N	-2.31972661118435	-0.80531342313606	1.08430240992368
H	-2.72969065818817	-1.09964369998059	1.95846802567138

3^{Nb} E = -2153.842877035704 au
 ZPE = 0.18846127 au
 G = 0.13671065 au

P	-3.16748295401845	-0.49432896691580	-0.35023460068735
Si	-0.40804909052826	0.59873512148346	0.94882742758784
C	-0.42109387255758	-1.34424609291853	1.50710302342487
C	1.01045768462934	0.27790112059229	-0.40217603781660
C	0.22499005159917	1.18711020588726	2.73260907418665
C	-0.60147243143277	2.52904920110704	0.31670993739769
F	-1.74644446182594	3.13547043389385	0.82234103836120
F	0.40216545846497	3.37128238154641	0.60323527979609

F	-0.77959416754349	2.58350401023694	-1.04251900433968
F	-0.35324291397846	2.34425675639946	3.13868350515953
F	0.01590065604338	0.30284270113538	3.73346457901437
F	1.56304159535901	1.41330665046461	2.68724302590354
F	0.69448708500496	-1.83178722352762	2.06689832234975
F	-1.43658310445813	-1.64537119525255	2.37396364063792
F	-0.67278089314921	-2.16145897211280	0.40306076888386
F	0.43402553251808	-0.08515615677835	-1.59699142477207
F	1.86064817845574	-0.71964843473417	-0.08560435178582
F	1.77319034492736	1.35472490127835	-0.66863604426793
N	-2.17888129735052	0.45989946396157	0.52634394014342
H	-2.60666257173335	1.37199042006778	0.64984040955234
C	-4.59958121359614	0.52452508349264	-0.75594201720542
C	-3.79455206006778	-1.94364445833215	0.51395615199099
C	-2.44380870049892	-1.04211485169001	-1.89985415712857
H	-4.27668303290446	1.40125722561534	-1.31763709486525
H	-5.09421506248697	0.84725274447696	0.16092804492902
H	-5.30715779115219	-0.04710246402596	-1.35664078517853
H	-2.11953488611227	-0.17268616515352	-2.47033394658326
H	-3.19019611419554	-1.60281721848664	-2.46487539583110
H	-1.58107854327978	-1.67398707663939	-1.70520675130235
H	-2.98980671286907	-2.64751584335368	0.70575629538732
H	-4.56047621917671	-2.41847660152115	-0.10194064812027
H	-4.22701578208595	-1.63589151019705	1.46554220517776

3^{Nc} E = -1252.203682853196 au
 ZPE = 0.11210578 au
 G = 0.07467423 au

N	-2.39802271440252	0.03268185043169	0.72959982822345
H	-2.94437559769350	0.80687091412790	1.07821393434967
P	-3.10741074372336	-0.91089860569287	-0.36363442738781
Si	-0.62415272955571	0.12246578803574	1.06575753285854
F	-0.51588621467178	-1.27298136343584	0.06618034475028
F	0.04053359028997	-0.68592206137092	2.28614404195623
F	0.35000339194945	0.91572520179715	0.05867216714780
F	-0.94716560626964	1.45988143923718	1.98094010794882
N	-4.68110679672340	-0.42896023847173	-0.46170570342114
H	-5.21064268560250	-0.74121242929784	-1.26114322088477
H	-5.22016675742283	-0.41787272172890	0.39154973602734
N	-2.63841846614515	-0.80771696504640	-1.94799510642242
H	-1.71011575631843	-1.18508948843809	-2.10004426217315
H	-2.71795046427127	0.11388851965549	-2.36047579702270
N	-2.96766822827275	-2.48134646024269	0.10335764121349
H	-2.07177662981964	-2.70237171567417	0.52165934805947

H -3.27424686134680 -3.18444715388567 -0.55396105522309

3Nd E = -2202.001697932964 au

ZPE = 0.15677221 au

G = 0.10599688 au

P	-3.16282178315115	-0.50126238019267	-0.32941395758999
Si	-0.47401168025783	0.61930593639624	0.95066412772240
N	-4.39013045791806	0.43718795552670	-0.89536289886904
H	-4.95365448108443	0.05893125013998	-1.64167332680122
H	-4.91748960032356	0.99937409340248	-0.24413786653111
N	-2.55433571168542	-1.12022187739788	-1.72237067406132
H	-1.85898027559385	-1.84388860571316	-1.59327879838568
H	-2.24650203462490	-0.44196051603502	-2.40816875450016
N	-3.61768816137171	-1.77714175754432	0.57718101439422
H	-3.14132593410254	-1.92144106655634	1.45623020281004
H	-3.95846607827021	-2.61563112769764	0.13387349105975
C	-0.40725054193035	-1.34478215198410	1.46900844523092
C	0.86650997519498	0.31073745151570	-0.48853149052549
C	0.18850593738375	1.16847789300802	2.73622224433407
C	-0.66503766039990	2.56272075608100	0.36552605465480
F	-1.79404438479979	3.16359404531603	0.90636319435945
F	0.35493977185028	3.38397282069628	0.66014278475581
F	-0.86302534936341	2.65572088365726	-0.98645288103134
F	-0.38819028680501	2.31372710872867	3.17318158125728
F	-0.00455328701450	0.26327348122933	3.72161094302126
F	1.52503963233494	1.39906611714884	2.67630606608640
F	0.74625272618910	-1.77709647294005	1.99371772459903
F	-1.37923350619697	-1.70430046853031	2.38129883261191
F	-0.65514754495264	-2.17055326368512	0.37851721444022
F	0.20660063543532	0.00587513601782	-1.66056070377540
F	1.70461472710981	-0.72210127855937	-0.26793788608217
F	1.64142543691269	1.37509363421203	-0.76252896681574
N	-2.25567082326386	0.48056467124967	0.58793946064644
H	-2.65523726930065	1.41377335250992	0.59911655298461

3^{Ne} E = -2310.374454746704 au

ZPE = 0.36775992 au

G = 0.31103932 au

N	-0.41868265253521	0.16776462651844	0.29972103914841
H	-0.70638124424313	0.59324467671907	-0.56767805113924
P	0.12868275803843	-1.40720781715446	0.18879939730515
Si	-0.38859862389400	1.27194441680558	1.69213268922431

Si	-0.78949017344774	-2.08186697284935	-1.79945426640144
Si	-0.66079240031483	-2.74857607376771	1.89640066860500
Si	2.42134249930732	-1.46683736067391	0.09005109860849
C	-2.62073650880781	-2.34474049097282	-1.51138271007647
C	-0.55539802151601	-0.66486745699139	-3.00597398468330
C	0.06180295619175	-3.63102365963370	-2.41927142187305
C	-2.32805585795910	-2.06834912182529	2.37887572204321
C	-0.79938150716628	-4.46764740225044	1.13558192081965
C	0.54857008060719	-2.87596081000355	3.31449458326806
C	3.09941977115457	-0.53765348026684	1.55364510685923
C	2.91259476927589	-0.64406684629841	-1.52137376926818
C	2.93388835463978	-3.27354667203691	0.09702451119672
H	-1.11852521456691	0.22268176729106	-2.71129326980990
H	-0.93204621988443	-0.97084473543665	-3.98622038577906
H	0.48951951326052	-0.38015845465938	-3.12523162787930
H	-2.83126083950488	-3.20293194324187	-0.87397883942363
H	-3.07103656917728	-1.46209501321192	-1.05346650849570
H	-3.11842351092474	-2.51138409356933	-2.47072778635410
H	1.10281673837335	-3.44100356228212	-2.68510219977229
H	-0.44751631738206	-3.98363649930050	-3.32039459036927
H	0.03665429345573	-4.43933946687348	-1.68866229041776
H	-1.53193552419301	-4.53232925348766	0.33160252257444
H	-1.10944523163555	-5.16747798628518	1.91703525574324
H	0.16084378495491	-4.82042679997252	0.75374911107171
H	4.02296064316476	-3.33652926850328	0.02000108237269
H	2.64440489052732	-3.77671227628203	1.02043524878371
H	2.51204431825337	-3.83066149077479	-0.74027330909920
H	4.19131713527868	-0.51684998570783	1.48437113994200
H	2.73421934098157	0.48903862212344	1.58438254230381
H	2.82040743293731	-1.00790064274213	2.49555760831436
H	1.51920204701088	-3.25834697552575	2.99509096277874
H	0.14559987978930	-3.58622123032785	4.04305007221364
H	0.68971387852312	-1.91421747035625	3.80077723213883
H	4.00030885724850	-0.53990926008782	-1.55991500813717
H	2.60469792999251	-1.22130124950076	-2.39455326890501
H	2.48460850655972	0.35726061838504	-1.59675221097173
F	0.20903597021155	-0.05240916969846	2.59002671510336
F	-1.64626054332574	1.38834845187457	2.69978564950566
F	0.93658615843993	2.12609274738419	2.05866583094314
F	-0.97605613616590	2.45331871736739	0.68358606461558
H	-2.23224260694779	-1.07400907677156	2.81410878775496
H	-2.78565445123076	-2.72928602229365	3.12067667933556
H	-3.00407608335495	-2.00608801285060	1.52508434628206

3^{Nf}

E = -3260.164845599747 au

ZPE = 0.41268415 au

G = 0.34359488 au

P	-2.24715799163697	-0.59462801455631	-0.61215530647489
Si	-0.09229641657864	0.72595632205042	1.70966253680324
Si	-4.49715928456333	-0.34577877084501	-0.13717129768088
Si	-1.87004631002014	-2.88127009900482	-0.78222723828843
Si	-1.84264044372742	0.46290345999726	-2.63127594093482
C	-4.90208086660350	-1.54847749842595	1.24045162712924
H	-4.19311845315581	-1.45510274495490	2.06487972324988
H	-5.89499565384649	-1.30964711075656	1.63217336132347
H	-4.91605883345333	-2.58834180330957	0.91579236163983
C	-4.71028823195209	1.40127633845857	0.50552860250886
H	-4.31744745821759	2.15848550115369	-0.17074452546687
H	-5.78269974925573	1.58153502859512	0.62742033131856
H	-4.24864037919581	1.55119688201098	1.48219186633629
C	-5.57281911029116	-0.61423492184162	-1.64641623222591
H	-6.61963744562236	-0.55329618281538	-1.33519799596681
H	-5.41336963857412	0.15640884901122	-2.40120636208566
H	-5.42358878547296	-1.58836083112714	-2.11005996294736
C	-1.73296919844566	-3.55920012339108	0.94878434227467
H	-2.63476367102678	-3.38111637412389	1.53330077755213
H	-1.57888895819529	-4.64056320353396	0.88581642848355
H	-0.89302012170489	-3.12678477007913	1.48729395950830
C	-0.36212577413037	-3.27880165749250	-1.81649296697726
H	-0.36880058602771	-2.76410810591945	-2.77825290150365
H	0.56460710668174	-3.03131782635479	-1.30412501470486
H	-0.36468755797462	-4.35368866120809	-2.02010886113974
C	-3.37399960774931	-3.59026292690848	-1.66170932233886
H	-4.29704850973247	-3.46713989046029	-1.09661680511070
H	-3.51868541103734	-3.16658946156935	-2.65570909051734
H	-3.21056523679518	-4.66458426167779	-1.78763288015996
C	-0.02671196322960	0.62964566356150	-3.02446459116462
H	0.05680606280015	1.11113022347636	-4.00381961471287
H	0.49901097656670	1.24461540598086	-2.29805380167457
H	0.47342682725896	-0.33643831044940	-3.07978981687358
C	-2.64892667570881	-0.63622591990159	-3.92625311614014
H	-3.70603785089767	-0.82079206117601	-3.74078872051654
H	-2.56753137201582	-0.13678913277179	-4.89605243625575
H	-2.14196385852121	-1.59791549830093	-4.01588148816918
C	-2.68046807378003	2.13538140933819	-2.56340591668992
H	-2.43669331013979	2.69125352560716	-3.47310165704852
H	-3.76650230429283	2.05114721095020	-2.50983858813437
H	-2.33223981236306	2.72228055730326	-1.71404655668099
C	1.45508503431335	1.39134642588929	2.81544796506238

C	-0.43962739479623	2.53908049898405	0.97337020403124
C	-1.08978182655761	0.10280277009440	3.32435681094758
C	1.07691088667283	-0.54325465251387	0.74722498318653
F	0.23918743115461	3.57083659799342	1.48968575481907
F	-1.75935308364194	2.88647096011404	1.06155407472612
F	-0.15224184763250	2.53305362477470	-0.37084913734035
F	1.08410859765086	2.28654584633415	3.77051113253534
F	2.42087757599973	2.01804258629101	2.08811386224769
F	2.08784672987108	0.37465778922881	3.47326010145795
F	-2.33416903013540	0.69779422612189	3.38014455720625
F	-1.33390230761887	-1.23548419913459	3.26233418004491
F	-0.53238895574200	0.32099984943429	4.51973885553311
F	2.37261845581124	-0.21925028122209	0.65132670014636
F	1.02962496343022	-1.77369393155909	1.33356165353448
F	0.66088580721977	-0.74236578715104	-0.54585357764571
N	-1.60545311810649	0.12604349842123	0.75028887751874
H	-2.37938847526303	0.54099674336067	1.25236180244558

3^Pa E = -1490.232914733634 au
 ZPE = 0.13713763 au
 G = 0.09732873 au

P	-1.17006706074242	-0.02120401154016	1.46115090825022
H	-1.74813022080433	1.19916180653039	1.03270362321193
P	-1.76769976674974	-1.01327280192642	-0.36063554412809
Si	1.10216732928673	0.35987238231040	0.96320448338416
C	-3.56113226983252	-0.81690703933052	-0.56561996246539
H	-3.80629822667299	0.24173134206004	-0.64960597528039
H	-3.89838139933271	-1.33435551056184	-1.46501477887988
H	-4.07439355549248	-1.22659280325991	0.30367323360542
C	-1.45223106116780	-2.78957665886217	-0.24691124987182
H	-1.82085104030797	-3.28882615659385	-1.14403498221670
H	-0.38005894437281	-2.94362722687582	-0.14566996713280
H	-1.96058812094067	-3.19171535061642	0.62899701810068
C	-1.01840924750442	-0.42154151804264	-1.89912131515305
H	-1.43169498384720	-0.96864857106280	-2.74855910102855
H	-1.22479670391508	0.64238315497135	-2.01332732646404
H	0.05908808552659	-0.56168557585860	-1.84552912433227
F	1.05948652534700	-1.21650498114399	0.34825717377355
F	2.26226223848897	-0.01757267686887	2.00461348658601
F	0.82617056025751	1.84385114687991	1.63265538700287
F	1.56972777277639	0.95263419979200	-0.46527310696180

3^Pb E = -2440.032721850929 au

ZPE = 0.18229909 au

G = 0.12933714 au

P	-1.65442891609861	0.87940629849225	1.43371788167898
H	-1.96866584014565	2.09911447082093	0.79016650310134
P	-2.27392779794276	-0.14656698175923	-0.37661677248385
Si	0.76974811569746	0.95495209943462	1.40849571757316
C	1.71612548962755	1.76385452562722	2.95381194384269
C	0.66809896819094	-0.84106929609964	2.37254506479102
C	-4.08580679710973	-0.01525132162440	-0.37498335492251
H	-4.37834118604483	1.03464507034195	-0.36786981283258
H	-4.49524818268602	-0.49602055951072	-1.26498636105094
H	-4.48452936972575	-0.49602454588569	0.51735135506693
C	-1.89650442442080	-1.91117537083560	-0.38948218467757
H	-0.83240281747536	-2.06024336265309	-0.55080992234869
H	-2.17330451560551	-2.35899684927041	0.56339295375196
H	-2.46466351529343	-2.37786831601116	-1.19573887874338
C	-1.74130766548625	0.54068681849921	-1.96293382617457
H	-2.24440250295505	0.00113411614219	-2.76784052832981
H	-2.00462448411674	1.59622000823276	-2.00639202879248
H	-0.66425904845028	0.44522113790356	-2.06692171118650
F	1.59716091335910	3.10533504716969	3.04242697723572
F	1.29697699407498	1.27425231092744	4.14395913426858
F	3.04411846650859	1.49557486494460	2.86306290238720
F	1.81849495525047	-1.24981689896981	2.94007476169596
F	0.29665452653481	-1.84803822773815	1.50617840119742
F	-0.27405531434496	-0.87931478442297	3.35650915715649
C	0.67092513090422	2.72638858731078	0.41993630638183
F	1.84315731229529	3.37897688648000	0.30248703169599
F	0.20450292165016	2.55671971763994	-0.86574112134433
F	-0.19596716947212	3.61576476853265	0.98937056193272
C	1.91374303286662	0.15110450012086	-0.01104110262275
F	2.76864174590831	-0.78083101644970	0.44429362152545
F	2.64455436835044	1.02203423253216	-0.72740826340395
F	1.10622416615495	-0.49634952992222	-0.93263949636960

3^Pc E = -1538.383998394767 au

ZPE = 0.10573767 au

G = 0.06739327 au

P	-2.79531448597346	0.02807321312124	1.54098949890831
H	-3.05265255332729	1.29070267562253	0.95126805331914
P	-3.27550269330736	-0.89561946633011	-0.34101627848741
Si	-0.45292711276885	-0.16602345248831	1.17649615628475
F	-0.75346214875000	-1.78981573457604	1.54137696350592

F	0.68310778210611	-0.07090086125745	2.30358343202318
F	0.03517193678869	-0.55563560651154	-0.32695054289681
F	-0.44663864461153	1.45412845167601	0.87586367370581
N	-4.88431676656567	-0.64715183176438	-0.62491550892185
H	-5.26596439771685	-0.93126632646918	-1.51594505730711
H	-5.51641341756016	-0.77016425087556	0.15126627989800
N	-2.64550909642028	-0.33239530517893	-1.77593263615575
H	-1.63576269984196	-0.42872049961317	-1.82545654976702
H	-2.93104474063359	0.60329550398481	-2.03540256372321
N	-2.82914582669342	-2.47109380743808	-0.22184802118176
H	-2.06627544437877	-2.65777712245121	0.42441456512212
H	-2.80591896034539	-3.02694106945058	-1.06467635432632

3^Pd E = -2488.186755460795 au

 ZPE = 0.15022336 au

 G = 0.09812203 au

P	-2.80396607705578	0.28339123800475	1.43977618046768
H	-3.23979701216874	1.54879766819957	0.99197151011440
P	-3.29292128470308	-0.54964519993853	-0.50665160480446
Si	-0.43130822444493	0.61601769196019	1.16758235982164
N	-4.70840304913100	0.17160976999608	-0.94073399771914
H	-5.08315093128042	-0.01515239588636	-1.85950196177885
H	-5.40301074957604	0.35646180535278	-0.23434913173508
N	-2.41764721618104	-0.34356274887591	-1.89457208060681
H	-1.54898421098880	-0.86193121283879	-1.93316218051238
H	-2.28112395513581	0.61601735734482	-2.18755885848223
N	-3.34682446243206	-2.17653862070264	-0.30137849067447
H	-2.96230244288187	-2.57038269559702	0.54326284593388
H	-3.32032868159145	-2.78666916298387	-1.10420831519107
C	-0.24748716088629	-1.22154680729409	2.03477676784803
C	0.65334567777895	0.01276085299773	-0.39094356674222
C	0.51906263147622	1.46471085473187	2.68880637536059
C	-0.80272327379412	2.42491457403408	0.31423031186868
F	-1.42607519695194	3.26481489521207	1.18690781781677
F	0.28596111470911	3.08080028047623	-0.13335802004623
F	-1.65576436623263	2.35412702122199	-0.77265654228223
F	1.09709564956812	2.64530405168635	2.38856897569071
F	-0.36428377460922	1.71256515700829	3.69605308306053
F	1.49408037911667	0.68962249651588	3.20863728820553
F	0.97810685155933	-1.77659084738763	1.98664573201469
F	-0.62037066770739	-1.20209483132302	3.33732465612995
F	-1.08912184546664	-2.16360707490739	1.45128184064124
F	0.30687151123499	-1.25794342318509	-0.78711058907759
F	1.96570303361946	-0.02246637062387	-0.09768994809252

F 0.52425359415653 0.76214257680147 -1.51285292722909

3^{Pe} E = -2596.579782248152 au

ZPE = 0.36150906 au

G = 0.30353246 au

P	-0.98376971743202	0.49098482865991	0.18498829577090
H	-0.12556075468867	1.10344377309316	-0.75686714778820
P	0.05304664787301	-1.46249237869642	0.10408163146121
Si	-0.22669691848854	1.57695304444084	2.09350206277117
Si	-0.79060723045304	-2.25732109318297	-1.87788855553067
Si	-0.70317372657008	-2.79607210356608	1.83526393391456
Si	2.34931790134604	-1.39285850869114	0.06974214921784
C	-2.62424780200807	-2.51898947103505	-1.60464481434121
C	-0.53487156290783	-0.93077441710682	-3.17451249284132
C	0.06823314918768	-3.84168491467916	-2.39555283686937
C	-2.35203449666665	-2.10063084150083	2.36200358233781
C	-0.87448730264215	-4.53342982471218	1.13789979546126
C	0.54120165696828	-2.87595614874937	3.22448981008825
C	3.00829703240689	-0.57558777210661	1.60286593126067
C	2.83132038673787	-0.44051698293258	-1.46845579839145
C	2.92499504536857	-3.17663964417558	-0.03835138969829
H	-1.07267798645040	-0.01781998678673	-2.91810169296101
H	-0.92429983244155	-1.29140761388810	-4.13089448896020
H	0.51572071373303	-0.67853155860300	-3.31697205463842
H	-2.84201986840607	-3.33009587870142	-0.91067382653115
H	-3.08810004411803	-1.60713639484809	-1.22561036629478
H	-3.09688570055303	-2.76341976652934	-2.56006413523474
H	1.10477274056141	-3.66068967630350	-2.68393065659750
H	-0.44601047272349	-4.25347857168304	-3.26866159426746
H	0.05665829766496	-4.60170892093834	-1.61518763787310
H	-1.60736408895623	-4.61612035126961	0.33667931466183
H	-1.19771510624112	-5.19414998955147	1.94776833647236
H	0.08046048070131	-4.91470051200384	0.77170341341714
H	4.01765634855970	-3.19265063027987	-0.08601071657335
H	2.62976790152244	-3.75055680976238	0.84134575926387
H	2.54605641689715	-3.68995017859115	-0.92147923447921
H	4.10141499095582	-0.62137157968363	1.56244433694467
H	2.71002396010125	0.46838685609970	1.67982156436013
H	2.6786943140402	-1.07663565731979	2.51113515967281
H	1.49208607560385	-3.30320758812011	2.90331681418416
H	0.13434015733518	-3.53553776838705	3.99749615425921
H	0.71524181303496	-1.89610864637616	3.66179772543328
H	3.91303118188851	-0.28073294253070	-1.46414717664993
H	2.57887570114702	-0.97463403685224	-2.38515767153375

H	2.35494332186027	0.54083587572442	-1.49566790441348
F	0.11128156590116	0.05563773047869	2.74996790327854
F	-1.26940614514287	1.90314065439855	3.27565735948839
F	1.29140527780148	2.07705347671894	2.33966098512320
F	-0.63131140402867	2.92708206478313	1.21097054332202
H	-2.22658640898318	-1.12464513425450	2.83045559486079
H	-2.80996181451849	-2.77270057383599	3.09339487313083
H	-3.04178354214181	-1.99729289616202	1.52338725231163

3^Pf E = -3546.376871915610 au

ZPE = 0.40671654 au

G = 0.33639067 au

P	-2.57091197992850	-0.64517106380112	-0.56889844309616
Si	0.34031724447385	0.88333601473580	1.98754413497874
Si	-4.86722811415273	-0.45389869605246	-0.38320395579869
Si	-2.08415379080606	-2.88598972465002	-0.87786693547771
Si	-1.97144808681013	0.51367523148320	-2.47976463987176
C	-5.39792446405844	-1.72059911230269	0.89091069334661
H	-4.83870652770057	-1.60371583848007	1.82003756777034
H	-6.45676570767560	-1.57116284694342	1.11960201218534
H	-5.27758473718052	-2.74601605908122	0.54068257962033
C	-5.26228983511460	1.27337344050233	0.20937873608265
H	-4.90333076689987	2.04111425952409	-0.47534666511974
H	-6.34952255664083	1.37243254677907	0.28291278390459
H	-4.82926916366264	1.46393364001971	1.18994228334136
C	-5.73544885511675	-0.75909875440468	-2.01892687752614
H	-6.81444484326265	-0.72802233567314	-1.84076479913756
H	-5.50674161451536	0.01690270549489	-2.75037676219656
H	-5.50229732789877	-1.72721213134835	-2.45965977688246
C	-2.12271017456821	-3.73417427208756	0.78591548679788
H	-3.08927310077285	-3.61942879639086	1.27721113066916
H	-1.95702619345003	-4.80388326695402	0.62574836100189
H	-1.34912353219008	-3.37243660475337	1.45916605211014
C	-0.43209352804800	-3.06827314779051	-1.73252777092030
H	-0.45468752176682	-2.67343749599304	-2.74885486150004
H	0.37419195133002	-2.58138852740530	-1.18951885577093
H	-0.19589080596306	-4.13435779920469	-1.80138446493216
C	-3.42513673751098	-3.62229776581684	-1.96754740627325
H	-4.40498661748758	-3.60918735165617	-1.49079034605794
H	-3.50547677601791	-3.12746743504814	-2.93464658023700
H	-3.16704555484232	-4.66916536037875	-2.15385345692178
C	-0.12872711636417	0.74188371309296	-2.62913756816606
H	0.06056859168816	1.21093729476106	-3.59999004669632
H	0.28375134360734	1.38857439308262	-1.85940556492528

H	0.40724717576884	-0.20552945362944	-2.60597334856213
C	-2.56084647432891	-0.55216200033390	-3.91026478880029
H	-3.62288410128510	-0.78690940075124	-3.86505970358499
H	-2.38612699741862	0.00693711067618	-4.83455981458227
H	-2.00346109872909	-1.48556415886021	-3.98742565200232
C	-2.88096939683333	2.14812269834816	-2.51706878852380
H	-2.51272467707696	2.71948087151223	-3.37433861842709
H	-3.95507500193161	2.01443555398467	-2.64985333812295
H	-2.70818321734090	2.74472075039308	-1.62339912580947
C	2.14239535151175	1.60948693406984	2.52174060392577
C	-0.10108033808213	2.56667668056390	1.02200205368484
C	-0.19810849890500	0.61087531110213	3.87905061995898
C	1.13367196977588	-0.69934057145701	1.11243711180265
F	0.94908619907654	3.17412847118040	0.43916792431902
F	-0.64866822973486	3.44881347344639	1.89005088998370
F	-1.01834047495912	2.41155795880650	0.01848439854283
F	2.07117156565645	2.88095058699574	2.99852710991630
F	3.01901183064177	1.65007257927552	1.47917350570974
F	2.75227354346456	0.88057823974458	3.49185416905611
F	-1.53734892572681	0.61175604112281	4.10581358557412
F	0.25095972945025	-0.60855233099829	4.27946675830203
F	0.31637259145677	1.52194565679463	4.72216343314196
F	2.35926832900520	-1.03644236543601	1.53904840888720
F	0.38588041790526	-1.82866864408667	1.23107211338030
F	1.23739406598711	-0.46210161230619	-0.23056728259451
P	-2.06151791985703	0.18350742419188	1.43538705924689
H	-2.07996500818354	-1.10217187760886	2.02376038127630

3^oa E = -1223.923772703803 au
 ZPE = 0.13129970 au
 G = 0.09227589 au

O	-1.28732015090332	0.98699228991570	0.97686059386462
P	-1.90875991243413	0.28165021954083	-0.22733348491363
Si	0.47154999187661	1.14786727856637	1.34045444984247
C	-3.69288121666594	0.35612113026642	-0.04267080787826
H	-4.00758886539947	1.39887403755831	0.00079779371570
H	-4.18540058903934	-0.13710021287907	-0.88148496441705
H	-3.97678513573974	-0.13835514400874	0.88641406726201
C	-1.40664719481126	-1.43965726704694	-0.31665736393193
H	-0.32222525996509	-1.47782499095369	-0.42145319010000
H	-1.68101470912445	-1.94196345720930	0.61066117846730
H	-1.88109192714549	-1.93526487004157	-1.16483203819670
C	-1.45024916430699	1.08053819669256	-1.76809451062113
H	-1.92758265686087	0.58653815082057	-2.61562234285576

H	-1.74911317692063	2.12793520669077	-1.72996413853538
H	-0.36606089679651	1.03588894936342	-1.87267848464793
F	1.21212565929063	1.90435378841771	2.55109403768883
F	0.28032376685162	-0.21503200627561	2.25047707960350
F	1.31294345344985	0.36821044453813	0.19130593324326
F	0.39773635464457	2.54399338604411	0.46091816241007

3^ob E = -2173.734507958363 au

 ZPE = 0.17593474 au

 G = 0.12369767 au

O	-0.45450097723995	0.37074144017125	-0.07448306664053
P	-1.92723243453691	0.17833653243227	-0.44160005358388
Si	0.85944482902632	0.93372428573005	0.95481357593732
C	-3.01543015532317	0.92798653580345	0.76519704919531
H	-2.80129800673094	1.99368511607382	0.83186118066741
H	-4.05368001776063	0.77574369605248	0.46634749515806
H	-2.84074509444693	0.47216143767688	1.73893719753074
C	-2.28500261523698	-1.57596419972651	-0.53411831012885
H	-1.62477511160980	-2.04056307756553	-1.26643244299558
H	-2.09711620062465	-2.02561351757411	0.44030925824317
H	-3.32449121297476	-1.73595262493028	-0.82386593173393
C	-2.21703287730804	0.92667202120284	-2.04401431268420
H	-3.25405462186817	0.78583709084597	-2.35155142179782
H	-1.98791847732428	1.99008387856413	-1.98012711083475
H	-1.55298203793471	0.46900145985134	-2.77757008911260
C	0.41717456407701	1.88544777891739	2.62379682217100
C	0.67193193699133	-0.88533452622412	1.78649980469053
C	2.80526575870698	0.71131530150945	0.67596639576116
C	0.72694420085239	2.58581987426010	-0.18320319671427
F	-0.53514105712768	3.14830619074946	-0.06272560017638
F	1.59079316788242	3.57984139949362	0.07423384970689
F	0.84747354090319	2.30884157513783	-1.51766941603627
F	-0.94854948996727	2.02568566189541	2.70747642177343
F	0.92602618433367	3.13032948509747	2.69638733459078
F	0.79447521705714	1.24779500731130	3.74763562266400
F	-0.57238956606949	-1.00723322261595	2.38490676096000
F	0.70130445396543	-1.89619608159628	0.86539062137939
F	1.56959324014677	-1.21227121236622	2.73013836707852
F	3.46910370847125	1.06965037051736	1.80518377899109
F	3.31832507762019	1.45072731002538	-0.33043759471555
F	3.15200284405037	-0.57092230672038	0.40971693065570

3^oc E = -1272.098530275307 au

ZPE = 0.09988382 au

G = 0.06205742 au

O	-0.72970884360502	1.12184339028732	-0.21863172327398
P	-1.80351574768805	0.17656566830255	-0.67766946811661
N	-3.38336985787787	0.40413473856113	-0.27843993286724
H	-3.83916851938733	1.20542004022748	-0.69041336447258
H	-3.61210193238830	0.28327762454172	0.69834393333662
N	-1.49424800495515	-1.30434592302985	-0.05899034215457
H	-0.57122928393480	-1.48631225309413	0.30575253746948
H	-2.11253933151607	-2.08779922417168	-0.17295486893724
N	-1.85182409425672	0.35072729223313	-2.31560907350598
H	-2.43524743987576	-0.25462515278449	-2.87060890752523
H	-0.98889946621837	0.62109307633718	-2.76171692328261
Si	0.24502566565798	1.35645677972888	1.43199254604398
F	1.08386452683453	1.56243912795955	2.80201101030243
F	-1.20662871299160	1.45235167763777	2.12569181427205
F	0.81357919278799	-0.13609575913834	1.15934620589263
F	0.88328764941506	2.60705710640165	0.67164370681891

3^od E = -2221.894710827301 au

ZPE = 0.14358453 au

G = 0.09138633 au

O	-0.42334002023393	0.37382852637435	-0.25843474062309
P	-1.90612398828260	0.17051214150858	-0.53969692085346
Si	0.82328012890218	0.93773310709005	0.84708475633996
C	0.29344388987511	1.93208773151263	2.46853199728655
C	0.54631268409359	-0.85187589630910	1.73173399075371
C	2.76940184508140	0.64241943554682	0.66692546761281
C	0.78937440164902	2.57677979694785	-0.31163532834491
F	-0.43578179702416	3.19924113408897	-0.20833767371897
F	1.70777755641257	3.52334427276190	-0.05594855819058
F	0.91169546979921	2.27968957338993	-1.64692277743969
F	-1.07847227453832	2.05006770637944	2.49162443542522
F	0.77792267274776	3.18631408277078	2.52768608937134
F	0.63421700688692	1.33256263731650	3.62521225458328
F	-0.71697437988290	-0.92614717582940	2.28864609362258
F	0.57525003112479	-1.89662873543557	0.83355860863704
F	1.40302937593403	-1.18456464446627	2.70764498911289
F	3.39126460725004	1.01962425863496	1.81376645107833
F	3.35122568659909	1.32907354190244	-0.33899325669895
F	3.08452679609576	-0.65929365879013	0.46083980880350
N	-2.19786857062352	1.02916444738070	-1.88948901794857
N	-2.10732231153836	-1.44279880131899	-0.60339745567591

N	-3.01318052461454	0.71638490987460	0.52416769729233
H	-1.321311103392070	-2.03572546699058	-0.38206599870849
H	-3.01406338767968	-1.87676707283667	-0.60992728149523
H	-1.41539048144250	1.34793960960071	-2.43986890925522
H	-3.10068115474336	1.05628423578014	-2.33141400678963
H	-3.05567963368310	0.24421651298012	1.41728053028571
H	-3.11049260424376	1.71935713013513	0.60648485553736

3⁰e E = -2330.252383571642 au

 ZPE = 0.35556051 au

 G = 0.29878874 au

P	-2.37122352456402	-0.64993798799987	-0.43458546898536
Si	-0.88972475182544	1.06024862060142	1.55778345913434
Si	-4.55712804354832	-0.15507431422930	0.07496394867183
Si	-2.01434169055879	-2.90857680803822	-0.62544626221716
Si	-1.67334095736399	0.47326800332845	-2.33122715428901
F	-0.18880598192560	0.17306865938321	2.74537487491283
F	0.52508983877769	1.69709231803187	1.10259554942038
F	-1.90156727140999	1.78702376965775	2.58854625365465
F	-1.64173638203038	1.88796589768728	0.26560837223249
C	-5.04048288166406	-1.28681573036970	1.48560793946259
H	-4.32459745904574	-1.21728045157722	2.30649656897062
H	-6.01846041523377	-0.98771029219091	1.87239756506200
H	-5.10961122180849	-2.33011330921605	1.17540004316083
C	-4.70871394818200	1.63447720730911	0.56540711443534
H	-4.42128173476476	2.30461021649041	-0.24330127736824
H	-5.75117368699126	1.83668395479215	0.82992432593011
H	-4.07901292377952	1.86601714639866	1.42440837241368
C	-5.52600330673008	-0.54461659391622	-1.48623891974749
H	-6.59250037817225	-0.40308839368314	-1.29052232510978
H	-5.25491501108726	0.12037705474521	-2.30772677063352
H	-5.38740635889031	-1.57325452716730	-1.82080236192558
C	-2.16286054155302	-3.58999085310159	1.10746421573963
H	-3.19018051324540	-3.58816230778555	1.47054800367548
H	-1.80235803824437	-4.62231713234347	1.12312753492658
H	-1.55433417408051	-3.00451456416117	1.79811381399342
C	-0.25091730513383	-3.07941752635636	-1.23105302291532
H	-0.12001620903335	-2.73401770241615	-2.25674638315958
H	0.42583676830821	-2.51450310583497	-0.58725109374125
H	0.05128819261321	-4.12941451930006	-1.19092986500021
C	-3.25762440095855	-3.68515955016548	-1.79337560280814
H	-4.27111038595065	-3.62813031696838	-1.39264848904276
H	-3.25277221570362	-3.22301430311075	-2.78056129320914
H	-3.01717161029499	-4.74409205642226	-1.92228667881223

C	0.17125518963377	0.69409571276430	-2.17779528095038
H	0.54661731867138	1.17009773761957	-3.08850279854450
H	0.42408241708797	1.32881514528734	-1.32907538669164
H	0.68935718387854	-0.25881608150988	-2.06304827933264
C	-2.11086810267056	-0.67767458319103	-3.75601084863569
H	-3.17846816530360	-0.90368313784377	-3.79137938159676
H	-1.85598306041388	-0.17947043577749	-4.69587019172717
H	-1.56209220757454	-1.61909265372823	-3.72702335057088
C	-2.58856235385044	2.08193973125416	-2.58035437626353
H	-2.22205777075490	2.54547537654720	-3.50139231688761
H	-3.66336256238269	1.93446218001268	-2.69708401558572
H	-2.40927599381704	2.76453725101353	-1.75266587087223
O	-1.43295230842826	-0.40655731451964	0.83381615082685

3^{of} E = -3280.054402228785 au

 ZPE = 0.40051231 au

 G = 0.33152762 au

P	-2.40772650594989	-0.50703480757042	-0.52628838963997
Si	-0.92818891537220	1.46967342279859	1.61977037259166
Si	-4.66863975167250	-0.37972697686825	-0.06535869420628
Si	-1.69766188867950	-2.71879423815000	-0.34657114139398
Si	-1.91957159148493	0.25810351065557	-2.66274251162890
C	-5.06524779491956	-1.55238345336838	1.33514104261975
H	-4.44882346698618	-1.34925189605137	2.21104518664917
H	-6.11187347500903	-1.41534404603221	1.62188755657165
H	-4.93436701332985	-2.59799275660559	1.05496886645077
C	-5.02154173055144	1.38579217829211	0.41054705237018
H	-4.76204048735207	2.09134775436916	-0.37690049796767
H	-6.09286611641661	1.47823918012122	0.61279123045536
H	-4.48699739298778	1.68549010079279	1.31171282385081
C	-5.56810070571860	-0.87233998665807	-1.63614433994467
H	-6.64397388042138	-0.86586428121281	-1.43985679976658
H	-5.38103394462431	-0.17200067967469	-2.45067512116547
H	-5.30371768630636	-1.87382861991930	-1.97607530374560
C	-1.86072894425284	-3.55660563432263	1.31231851025978
H	-2.81070031936808	-3.35135172963466	1.80152633035003
H	-1.80720949612365	-4.63325874582908	1.11906200522143
H	-1.06081333064151	-3.28782537488366	1.99556907952590
C	0.05059084530429	-2.79897882991394	-0.99866231508558
H	0.10293504880483	-2.57339495036456	-2.06391227133536
H	0.70529226929188	-2.11101398063335	-0.46329112027929
H	0.43827141792911	-3.81093130498667	-0.85256330106821
C	-2.91727640836018	-3.56863341572643	-1.50283233601917
H	-3.91162195795760	-3.62619592474550	-1.05738684783826

H	-3.00700320796628	-3.12067232965071	-2.48899724572695
H	-2.56932845832218	-4.59684801760861	-1.64083517550508
C	-0.07565160425376	0.53234854288150	-2.69319533427163
H	0.18106427155162	1.04463595248745	-3.62517485208799
H	0.25906522081096	1.15743131546226	-1.86863148839281
H	0.47876140789763	-0.40519190172016	-2.66363855413626
C	-2.42613969144646	-1.00026956681788	-3.95691140122005
H	-3.47825945803677	-1.27925793311373	-3.89444275177311
H	-2.26724687576390	-0.54322491754218	-4.93827460205273
H	-1.82042380240331	-1.90583653859601	-3.92018848033748
C	-2.88484709937083	1.83875832618365	-2.89517456648504
H	-2.58797035928273	2.28492331919001	-3.84900673201781
H	-3.96068506694468	1.66295035977775	-2.93476108961217
H	-2.67571795276787	2.56274577097389	-2.11075368739536
O	-1.69738478483813	0.60106929664991	0.36201781631523
C	1.03764468508691	1.63500674818531	1.50132676839048
C	-0.78854906497544	-0.27866872671127	2.59539783175109
C	-1.78394601397854	2.34056031355188	3.19302296958946
C	-1.22998749702255	3.10740305821724	0.48463128689753
F	-2.01549660633184	-0.90571202864595	2.68325204672062
F	-0.00140659749211	-1.16552974261375	1.88900382725676
F	-0.29387175858544	-0.27446674171300	3.84381990240910
F	-2.74496194214557	3.24077991468346	2.86553805946535
F	-2.38416028257473	1.47583666127967	4.04864957308300
F	-0.85211978720919	3.01178068886761	3.91518824378903
F	1.45333533385607	0.95419098176791	0.38253442258360
F	1.70829195208125	1.09271701118494	2.54047263720550
F	1.50050360241141	2.89349204609761	1.36777008657375
F	-0.87230833048229	4.27415472057530	1.06079918521636
F	-0.54108763611196	3.05227429520957	-0.70232477078095
F	-2.54085668223269	3.26761369762855	0.10923509871707

3^sa E = -1546.519454778616 au

 ZPE = 0.12865797 au

 G = 0.08776538 au

S	-1.92425213784255	0.80298573852680	1.71502255617943
P	-2.27877196650544	0.14945837667457	-0.09365088711583
Si	1.42800034618617	1.43095073828573	1.43248788987369
C	-4.04808281547595	0.14020307591728	-0.52080661631148
H	-4.43217347045283	1.15743115736167	-0.44890916774623
H	-4.21049326733848	-0.24251300386136	-1.53008164619506
H	-4.58091059243848	-0.48191823724080	0.19776739425811
C	-1.72159578491316	-1.55661940056687	-0.39188165589674
H	-0.64643182372918	-1.60544783096822	-0.22502609181556

H	-2.21568941209580	-2.21802167088930	0.31926612482556
H	-1.95076542632387	-1.87587851250188	-1.41050587667617
C	-1.50122072975524	1.11961034160468	-1.42341596798535
H	-1.81504848441935	0.75729125447739	-2.40412979518652
H	-1.78412598816787	2.16538178992191	-1.30966922641586
H	-0.41888434635784	1.04170615079343	-1.33977248325102
F	2.97561102787634	1.72864023939932	1.36664638934915
F	1.06868354587296	1.23958178862896	2.94388111228976
F	1.18968358433405	0.12805705654606	0.57944721392009
F	0.69842611154660	2.65286607789060	0.77152270390003

3^sb E = -2496.293377127565 au
 ZPE = 0.17408388 au
 G = 0.12171177 au

S	0.02153942912429	-0.20541883918331	-0.90474368889702
P	-1.97577573071642	-0.03044900213228	-0.67399235567825
Si	0.99050290006624	0.97855169928207	0.99054693218129
C	-2.55330933197460	0.86208966692930	0.78420151908211
H	-2.19872648084396	1.88977194869154	0.76194567138941
H	-3.64500668502063	0.85945408239828	0.77342602190505
H	-2.20387544594958	0.36783115588979	1.68800938567971
C	-2.71576898428349	-1.67795435199764	-0.59090886090338
H	-2.42449202161735	-2.25068559255354	-1.47082008651759
H	-2.33919913402182	-2.18233955435567	0.29827751936786
H	-3.80366469499782	-1.60367098860239	-0.54495361154487
C	-2.67969478253390	0.80820908529403	-2.11270189685188
H	-3.76754999315363	0.84951852733565	-2.03638196216948
H	-2.27091465667380	1.81662380691091	-2.16058634855629
H	-2.39630620623830	0.26956910157563	-3.01661705121325
C	0.27920010918331	1.96076321251463	2.57889894842167
C	0.84321683562607	-0.80647845262131	1.90715594856106
C	2.95663128361761	0.92990049728419	0.88476086716629
C	0.82425639429366	2.59370967030739	-0.20091710741793
F	-0.46865108415077	2.86908432108930	-0.58592704010485
F	1.27572212608475	3.71943300316630	0.38799081684777
F	1.52380859405191	2.45495091605104	-1.34931275356810
F	-0.51411847415735	3.01421681372653	2.25221662967882
F	1.29021940688522	2.45008110866700	3.32756024540647
F	-0.48289026356058	1.19108894549386	3.39805979670933
F	-0.44705611849551	-1.27135698238739	2.01459767590673
F	1.52748444248010	-1.77564854251569	1.25737468874935
F	1.32728389972876	-0.77589883820269	3.16559124880904
F	3.53985191794932	0.29520228515958	1.92086635285518
F	3.51700422398251	2.15410999475200	0.81578035218600

F 3.32779729531584 0.26342398203274 -0.24239793748031

3^sc E = -1594.673160773300 au

ZPE = 0.09699595 au

G = 0.05736098 au

S	-0.31945345605678	1.52242039653422	-1.21708793805281
P	-1.77981891827525	0.24492130555329	-1.09827637141398
N	-3.22604469105617	0.58133140763818	-0.32417159805650
H	-3.76574556255969	1.30896358901437	-0.77308523863982
H	-3.11850199329812	0.76156298228285	0.66539571698691
N	-1.32291072218326	-1.08697062439881	-0.21101748841282
H	-0.34660012574966	-1.33259132024468	-0.21959133986671
H	-1.96001285062176	-1.86131739892621	-0.10242029730318
N	-2.37647173208070	-0.08767728857506	-2.61995388079779
H	-3.06723782045476	-0.81595931722045	-2.72826967867841
H	-1.71360463705775	-0.02859453637009	-3.37641389656059
Si	0.39361138355835	1.33679175850012	2.18836514797962
F	0.73904592239719	1.23527611144281	3.72368873101943
F	-1.17515366093649	1.26809961917810	2.08831923463196
F	1.09011209403741	0.11923135872246	1.48415165297304
F	0.94606257033797	2.70670016686875	1.67011439419170

3^sd E = -2544.453139298391 au

ZPE = 0.14179161 au

G = 0.08904310 au

S	-0.95554068084358	0.60696011677978	-1.13172543696306
P	-2.69031073162365	0.25013291529963	-0.25178698074506
Si	1.23724855611662	0.98361727600747	0.70467861074689
C	0.06485823602858	2.19958130909879	1.71167227770387
C	0.94534606141071	-0.94472643433558	0.97860333222037
C	2.84236169875414	1.19633089925262	1.83144636037591
C	1.97007091119892	1.65201546809258	-0.99437511426665
F	1.46184884097275	2.88020758704625	-1.24682630500504
F	3.30886815665347	1.78678299601121	-0.92294454595291
F	1.72661896222307	0.87934323393836	-2.06684870250973
F	-0.96386807101029	2.76751192622107	1.06156352864216
F	0.78028718787721	3.21018946779426	2.23988383986831
F	-0.47013957480279	1.50556032195497	2.75802508713309
F	-0.31641206070048	-1.25139624984260	1.36915553805399
F	1.20677966123649	-1.64630888274750	-0.13974509415833
F	1.75000479708304	-1.43247073183019	1.94316989654429
F	2.56442167362477	0.97764574976296	3.14108333647911

F	3.38727938238003	2.43072443431115	1.75461203301147
F	3.81449338229856	0.31995871831182	1.48309606625455
N	-2.96194860193862	0.32081434031057	1.38168438125348
H	-2.90183494958968	1.24385110959228	1.78712141418795
H	-2.46251315453086	-0.36429355425840	1.93100283047969
N	-3.09583600382967	-1.32460884294656	-0.54692372777977
H	-2.67781278775098	-1.78097841286773	-1.34042663683156
H	-3.97971717389067	-1.69915721617022	-0.23889896015576
N	-3.76118485261667	1.40057512328518	-0.77303102932851
H	-4.73958035124664	1.32908137489768	-0.53784922505049
H	-3.56095231348369	1.85906915702991	-1.64682247420843

3^ee E = -2652.837752758053 au

 ZPE = 0.35321967 au

 G = 0.29546939 au

P	-2.36808761316513	-0.71910407337883	-0.40012609710719
Si	-0.79136838205086	1.77002142966800	1.59432554403190
Si	-4.55341481077625	-0.23955027672122	0.12062927168415
Si	-2.07588765802085	-2.98481693202089	-0.69705716094604
Si	-1.63247940030375	0.39726016233206	-2.29536837452885
F	0.07283835888842	1.19247265403173	2.86864866446455
F	0.46863158627266	2.52858161776104	0.93336085292915
F	-1.76338963287602	2.67217717324602	2.50952642185741
F	-1.72544133984402	2.04319366745511	0.23054784217650
C	-5.06955091436531	-1.47347441256857	1.42978080640275
H	-4.35106743490146	-1.49805864705425	2.25064416029381
H	-6.03714894182005	-1.17531700549608	1.84262207384610
H	-5.17652058101598	-2.48257546288393	1.02983052454129
C	-4.67195648264027	1.50495493858606	0.75537513503023
H	-4.34241077003754	2.23343655845614	0.01643444058040
H	-5.71732340038417	1.70999341461274	1.00575567036327
H	-4.06931198386186	1.65541533037679	1.65082612764588
C	-5.54292582856788	-0.47437010026172	-1.45713641899806
H	-6.60179851004096	-0.30107659242849	-1.24557455348520
H	-5.24530288276271	0.23316427308905	-2.23201366270266
H	-5.44806460895176	-1.48245971365952	-1.86204051298377
C	-2.26399815428231	-3.82540973778462	0.96102027790596
H	-3.27349157891183	-3.73997803417068	1.36094513217924
H	-2.04132949774108	-4.88945199713563	0.83691904826315
H	-1.57074051756640	-3.41651982426869	1.69588543507091
C	-0.32418471282009	-3.21043777192383	-1.31751075404921
H	-0.16476060369109	-2.80254566833427	-2.31501151803077
H	0.38366209738552	-2.73719458434498	-0.63501972059751
H	-0.09111300439167	-4.27831854714091	-1.35298676703278

C	-3.35537230812042	-3.64283143805639	-1.89949784522496
H	-4.36185086298567	-3.57856933793923	-1.48248918630997
H	-3.34717281761998	-3.12570341506465	-2.85802188342742
H	-3.14887439424958	-4.69984523022534	-2.09012755144069
C	0.20062349884415	0.64121073672965	-2.07436857869118
H	0.62673920187960	1.01155527145778	-3.01137291684918
H	0.41357464267218	1.36807851479475	-1.29149173248373
H	0.70595488105473	-0.29162617006233	-1.82123654953295
C	-2.00874724988120	-0.74578685800232	-3.74272535191165
H	-3.07757995511299	-0.94908153194729	-3.83196910688640
H	-1.69916776689103	-0.23972715502058	-4.66193778837841
H	-1.48019444858469	-1.69701759138430	-3.70038748040363
C	-2.57544307940659	1.98189358053477	-2.59187032212036
H	-2.20653551952385	2.41810934158518	-3.52544579353041
H	-3.64512634780647	1.80855580132915	-2.71706182425303
H	-2.42098679363136	2.69879637541752	-1.79007886917747
S	-1.15337241739155	-0.45226330218388	1.27952993181699

3^{sf} E = -3602.634836711979 au

ZPE = 0.39848834 au

G = 0.32832835 au

P	-2.32811815559220	-0.52931317600068	-0.89499398556028
Si	0.24573888454143	0.93301587932254	2.10301684124159
Si	-4.49275074186150	-0.29013442891806	-0.11313638811399
Si	-1.70200037311691	-2.75914243726119	-0.87965496424054
Si	-2.27355231081338	0.14777014449166	-3.10778800120533
C	-4.77481844136602	-1.38215271188177	1.37977370932845
H	-4.12019580457353	-1.12144179770195	2.20813886850721
H	-5.80884220374790	-1.25010158126496	1.71182480070888
H	-4.63709194998051	-2.44008619433124	1.15162492678855
C	-4.69362602642823	1.51659192228384	0.30324078334493
H	-4.60292283516867	2.14986285749198	-0.57913582102900
H	-5.68509249212951	1.67662021087389	0.73643638197011
H	-3.94449927441429	1.83883330009714	1.02488180137193
C	-5.67549943290977	-0.80655084264203	-1.47853951026481
H	-6.69818192739064	-0.71562775674605	-1.10112681306977
H	-5.59698175054051	-0.17271433044860	-2.36197386176347
H	-5.53113406483195	-1.84279198406482	-1.78491677545880
C	-1.37918226082415	-3.47632580120898	0.81124892541226
H	-1.20000122853229	-4.54753168150759	0.67339908506997
H	-0.50525143368927	-3.04614368213246	1.29245480903314
H	-2.23129082759490	-3.36371648070061	1.47995294792344
C	-0.20967092730177	-2.94713309335209	-1.99291539977436
H	-0.45476125866870	-2.76899827600193	-3.04020866064301

H	0.59755196391935	-2.27499752232458	-1.70484236073343
H	0.16286878324978	-3.97206312511672	-1.90993875254819
C	-3.18759733106336	-3.64981441276220	-1.61243528624803
H	-4.04325437291183	-3.63193615271679	-0.93617227305197
H	-3.50281691219017	-3.25569837325702	-2.57671572710607
H	-2.91220511881473	-4.69865556189765	-1.75839545488318
C	-0.48022712339501	0.36045099010131	-3.58586887471000
H	-0.43748119272829	0.79980481832673	-4.58701198361746
H	0.03240072311625	1.02762559992516	-2.89411853237791
H	0.05991639703849	-0.58494391450260	-3.61292252438671
C	-3.10189503027390	-1.09563749378611	-4.24496183747121
H	-4.13214492848539	-1.31173797148586	-3.96294991917760
H	-3.11802435950867	-0.67383163767761	-5.25435345798446
H	-2.55311722490155	-2.03656757707967	-4.29704497323882
C	-3.16541569107189	1.79176188532062	-3.17120019952391
H	-3.03602239193092	2.22717286558228	-4.16598801993261
H	-4.23619947882398	1.69518790129562	-2.98969874420163
H	-2.74906768277258	2.48715022279359	-2.44188383254317
C	1.32643613944828	0.98845934408924	3.76745422544022
C	0.20750056269842	2.88032128469843	1.76773641619327
C	-1.35607587097945	0.13345398636517	2.92608248719795
C	1.51773849371556	-0.14609841954340	1.04832841683652
F	1.00350729568537	3.55538878825847	2.61985607428827
F	-1.03787032865466	3.38266158623287	1.92509259754234
F	0.62106596799737	3.20895346497655	0.52467733120650
F	0.73085997640590	1.72400652563098	4.74116320325108
F	2.55961787883971	1.51915211694962	3.58641383853648
F	1.51891262603685	-0.25229060486285	4.29007709526717
F	-2.43911502312682	0.93833806317730	2.83307188260233
F	-1.69019961999923	-1.04011022606208	2.32477315536269
F	-1.21397915761045	-0.15363436082319	4.23214267432654
F	2.59323512688765	-0.54028950566143	1.75692784821310
F	0.95342229884909	-1.28909733849074	0.57212568669790
F	1.98979768671861	0.53499088657037	-0.01540220017430
S	-1.13108376442756	0.97355333936051	-0.14605578862860

4a (Me3P) E = -460.426855216622 au

ZPE = 0.11211418 au

G = 0.08286035 au

P	-3.51794290633782	2.39166804801661	-2.37640658575280
C	-2.64009422896364	3.20584890941021	-3.78814287803255
H	-2.93662224375513	2.73028790812451	-4.72469219827240
H	-2.93188767806661	4.25610299160217	-3.84200530457186
H	-1.55235373886317	3.14643150470926	-3.69175127040055

C	-2.63920772461692	0.76246006054937	-2.37638878122464
H	-2.93240683108868	0.18903191239498	-1.49526760560592
H	-2.93239175978126	0.18902053323522	-3.25750759101039
H	-1.55177787333177	0.87833496794045	-2.37638027324371
C	-2.64012173286942	3.20586357487914	-0.96466136290320
H	-2.93190931190686	4.25612042493460	-0.91082142889868
H	-2.93667530302463	2.73031835019151	-0.02811205667947
H	-1.55237925739409	3.14643761401198	-1.06102619340381

4b ((NH₂)₃P) E = -508.570444345650 au

ZPE = 0.08006974 au

G = 0.05181039 au

P	-3.70570339261341	2.34383342679947	-2.45770269282623
N	-2.87604046468458	0.86729240127223	-2.61439002600280
H	-1.86764340360497	0.85037307984139	-2.51681340204114
H	-3.32594455218345	0.05632761513483	-2.21883915597949
N	-3.17103643032960	3.22588707095811	-1.10473698420420
H	-2.17641534207457	3.31835177349173	-0.93411996635457
H	-3.70867662529831	3.11855028963296	-0.25863826006907
N	-2.66728507580769	3.18312277337105	-3.56520092329164
H	-2.71461651988228	2.79166207175089	-4.49772281392055
H	-2.88322459352104	4.17155784774728	-3.60596853531023

4c (Tms₃P) E = -1566.786988456767 au

ZPE = 0.33736810 au

G = 0.28819515 au

Si	-1.74873925258041	1.50625488828865	-3.26610775909734
Si	-4.66548572639580	0.61447287820141	-1.40721333963615
Si	-1.61957581226354	-1.18201043566440	-0.91177693914613
C	0.01259381867857	2.14359559363192	-3.09699815714693
C	-2.82867472487061	2.92994549156175	-3.85715780895050
C	-1.77821018663821	0.14246822486367	-4.56541696259541
C	-5.46278317920561	2.30775336772984	-1.22386750505180
C	-5.26368183038214	-0.46753106617241	0.01203952647390
C	-5.23594896899222	-0.14761039193323	-3.03171878249869
C	-2.47405619218841	-2.52753748099491	-1.91503856589999
C	-1.78513550683982	-1.58700451128500	0.91758720466617
C	0.21211299198841	-1.17661480914684	-1.34652277319578
H	-5.19098870810870	2.76061126296369	-0.26823432309202
H	-6.55246689784009	2.21928920024062	-1.25956669740573
H	-5.15639622242313	2.99277142043188	-2.01537076602331
H	-4.98193338023041	0.48147887697020	-3.88603586069277

H	-6.32382828736094	-0.26387601984469	-3.02121901018471
H	-4.79578264814446	-1.13171772327518	-3.19525910077654
H	-4.92111254575834	-1.49928463481313	-0.07643294527281
H	-6.35720576140993	-0.48256989900397	0.02590731668689
H	-4.92321061918667	-0.07967599473533	0.97409626807338
H	-2.86166729687183	3.73164438858050	-3.11681675843526
H	-3.85361010071903	2.61901309824293	-4.06379753510221
H	-2.41641066424261	3.34484902423743	-4.78140419897986
H	0.05697229709046	2.96656882053921	-2.38081947816654
H	0.37756173413029	2.51240799778757	-4.05991975618260
H	0.69738281271830	1.36699123919724	-2.75442038781582
H	-1.10664810803255	-0.67792897455546	-4.30765487576388
H	-1.45050671480515	0.54454943782719	-5.52872780389331
H	-2.77798702676668	-0.27160431127923	-4.69918022680904
H	-2.43191136924020	-2.32356927639233	-2.98539553345303
H	-3.52276762520741	-2.63851493422418	-1.63617986139510
H	-1.98290201526562	-3.48891368141069	-1.73728442768693
H	-1.36544473049064	-2.57471798605597	1.12904902241836
H	-2.82601495833995	-1.58922576542036	1.24330406784205
H	-1.24832335131497	-0.85435585290098	1.52363142519132
H	0.73948158255284	-0.37388372618066	-0.82775103098728
H	0.38506080022937	-1.05791061739473	-2.41704591917397
H	0.66421204694136	-2.12491541367143	-1.04220986720409
P	-2.43501505221329	0.90338278505935	-1.20057454363637

5^ca (CH₂-SiF₄) E = -727.466653728464 au

ZPE = 0.03935832 au

G = 0.00809705 au

Si	1.94585176744339	0.11085676208984	2.78657843559431
C	2.04261864083259	1.97300683766512	2.88325572254922
H	2.69199190290298	2.30145862418140	3.69913940872809
H	2.43344074961797	2.39229986770129	1.95185629086017
F	1.29145191737059	-0.51165751870724	4.07941792967223
F	1.08484864870268	-0.35176479626087	1.54718159408998
F	3.40729251065801	-0.47733267967236	2.63188018023973
F	0.76095337247173	2.49382199300281	3.09919215826616

5^{si}b (CH₂-Si(CF₃)₄)E = -1677.240424817588 au

ZPE = 0.0824453 au

G = 0.03531632 au

Si	1.80962081006640	0.27031836163301	2.81388859469974
C	2.29394824764715	2.10181033973123	2.94939031731744

H	3.02839703540623	2.21730885888123	3.74844280166098
H	2.74845323074768	2.43030505659802	2.01270614294526
C	1.26576955130650	-0.62368234662680	4.46024031845636
C	3.62804834706530	-0.42650927384939	2.57211345165276
C	0.96651896260747	-0.35424410267050	1.16728989889794
C	-0.48612777386673	1.33219537936934	3.06935678422423
F	-0.24956135822032	-0.91318568132277	1.36486884754453
F	1.70574360665066	-1.25769991830826	0.50252904393690
F	0.78488506237492	0.70119196267227	0.32980436406963
F	3.72524629313089	-1.76158927827261	2.44181072176135
F	4.19796188262883	0.12397793387926	1.46297170424244
F	4.42492741628344	-0.07186682408139	3.61769339354363
F	2.14278064359638	-1.56070576943068	4.86216159962950
F	0.05943390940038	-1.22638191209957	4.36591892350881
F	1.17542094928698	0.28762040916820	5.46398593986666
F	-1.13619359992105	1.55633365561793	4.15431710235130
F	-1.14895296270415	1.87399035247814	2.10948011438591
F	1.22214975651294	2.96700804663332	3.23192462530450

5^{Si}a (SiH₂-SiF₄)E = -978.547477899982 au

ZPE = 0.02992513 au

G = -0.00277100 au

Si	1.92479941378951	-0.15128716711925	2.78155155630965
Si	2.03124399037112	2.18892448860143	2.90278568114573
H	2.89863689009778	2.62316483272998	4.01741593951330
H	2.53426830983088	2.72154606042954	1.61944593255805
F	1.25057518230221	-0.81970118598278	4.05146157892664
F	1.08941658903633	-0.61615549070788	1.51536278768310
F	3.38567109126062	-0.76105011883880	2.64309117854880
F	0.54383804331148	2.74524767088773	3.14738706531461

5^{Si}b (SiH₂-Si(CF₃)₄) E = -1928.326343 au

ZPE = 0.07235050 au

G = 0.02347071 au

Si	1.90517378978728	0.14876751936469	2.78073219592445
Si	2.39910690992946	2.44750141364594	2.94682180318063
H	3.14883153486760	2.69601658753403	4.19269026940824
H	3.15724883253530	2.87888406852740	1.75792914077011
C	1.26348684136439	-0.70844748043865	4.41942479237291
C	3.67794198435851	-0.63892152700564	2.55471822489419
C	0.96686898371942	-0.42183441871479	1.16187000515623
C	-0.68843824650182	1.32734223143895	3.13526969566658

F	-0.17146966806674	-1.10129866883512	1.40521606943505
F	1.73829998976818	-1.21092649140998	0.38761896072128
F	0.63344419399821	0.65778771643232	0.40866823451746
F	3.70863898490030	-1.97717936192861	2.43353802366171
F	4.28557133587995	-0.12208858279056	1.45426914615477
F	4.46770205681326	-0.31193635111534	3.61321802960054
F	2.13192180526843	-1.63066792586743	4.87850114934566
F	0.07213458700671	-1.32418069436913	4.28400658414454
F	1.12197884878060	0.21749895966221	5.40349002422588
F	-1.23083830410934	1.64038701246597	4.26406157451787
F	-1.46186405269419	1.79265680217627	2.21430520795521
F	1.03272960239437	3.30683444122744	3.00454555834647

⁵Na (NH-SiF₄) E = -743.453277 au

ZPE = 0.02740803 au

G = -0.00364512 au

Si	-2.15122578834420	1.22900081788442	-2.77208962426298
N	-1.85176583418536	2.83937502289480	-2.24234150933074
H	-2.24999026127625	3.63130236735347	-2.73303925779339
F	-1.77044439939236	1.21235654230676	-4.29983527756084
F	-2.27131363439210	2.98519085290346	-0.89050879284585
F	-3.63889419033301	0.73243567278324	-2.61345497573334
F	-1.23525399207661	0.24261237387375	-1.96468580247277

⁵Nb (NH-Si(CF₃)₄) E = -1693.225945 au

ZPE = 0.07066973 au

G = 0.02379228 au

Si	-2.45094877221794	1.29813824529225	-2.65307580016112
N	-2.47556243270316	3.02881472548398	-2.84005020806535
H	-2.63793332512831	3.47208602562030	-3.73488906260308
C	-4.04865947058110	0.18137349275982	-2.84512036347115
F	-5.12989885506271	0.97122346864636	-3.07882333253334
F	-3.98087244801935	-0.70185012272861	-3.85204670066450
F	-4.32309978138910	-0.52767870272988	-1.71990852334956
C	-3.36696905861486	1.89883339776950	-0.60633485228393
F	-4.60808705697598	1.94067752192502	-0.30670001021804
F	-3.23546083365630	3.80044484782783	-1.91168891539157
F	-2.69224843965732	2.29087525840025	0.40617264635227
C	-1.59674088963115	1.09458951790226	-4.42313050045964
F	-1.46315785469843	-0.17754615406579	-4.83855428540867
F	-2.32009826290796	1.74526095269985	-5.38623200478805
F	-0.35792805374188	1.64688844242203	-4.44627156576068

C	-1.07950834946590	0.45210567367954	-1.54916198004696
F	-0.33683091648958	-0.43535222529975	-2.23038784612016
F	-1.61339324862071	-0.21674201394360	-0.49049599088249
F	-0.23640106043788	1.37778093833843	-1.03659545414360

5^Pa (PH-SiF₄) E = -1029.756213 au
 ZPE = 0.02178013 au
 G = -0.01058562 au

Si	-2.11076407304541	1.10576653331626	-2.84101637462020
P	-1.54214129994818	3.17422101599153	-2.11201487412128
H	-2.63712528128091	3.75142993816018	-2.81904461328071
F	-1.70954528397945	0.98113275400037	-4.36968366937364
F	-2.22492918482292	3.09214613321392	-0.64320617850791
F	-3.64625957637295	0.74405243590555	-2.70923785939668
F	-1.29812340055008	0.02352483941211	-2.02175167069948

5^Pb (PH-Si(CF₃)₄) E = -1979.534688 au
 ZPE = 0.06455751 au
 G = 0.01626284 au

Si	-2.34845170236528	1.24480352837083	-2.75877009429782
P	-2.27656980480444	3.53382320223820	-2.93598185166816
H	-3.38479801032873	3.49698529854051	-3.82774477555619
C	-4.02694892752323	0.24462161887706	-2.90027725199343
F	-5.07177368823455	1.09729888096035	-3.04944497902698
F	-4.04319704839536	-0.58480866257327	-3.95842794762850
F	-4.29145708282720	-0.50824764757820	-1.80806413349909
C	-3.41410155577132	1.86106148772237	-0.45719912199186
F	-4.66597164650454	1.98153026984192	-0.19465504293512
F	-3.10195267990174	4.00645195830721	-1.60476138638872
F	-2.76751385078411	2.18245890775299	0.60700604608587
C	-1.51035944046884	0.90335561643341	-4.50489236536047
F	-1.36724285646262	-0.38558644122812	-4.85368976822959
F	-2.23125697835173	1.50624581335949	-5.49438989880502
F	-0.27278725155235	1.46551100010399	-4.54356010432295
C	-1.05144796110537	0.41889813639925	-1.55272162127486
F	-0.20329176887429	-0.40781592597628	-2.18871733950581
F	-1.62249437083250	-0.29898181423536	-0.55793050664945
F	-0.30218248491141	1.38231806268345	-0.95907260695148

5^Oa (O-SiF₄) E = -763.2806876 au
 ZPE = 0.01504709 au

G = -0.01577122 au

Si	-2.21304853298331	1.03420511438606	-2.60431648333610
F	-2.24812434737258	1.31677293768871	-4.14520232685991
F	-3.65369260604445	2.92909745376985	-2.11867187369813
F	-3.34141575919958	0.00378395394104	-2.26018593003631
F	-0.81076552971758	0.48379962327462	-2.17107741904446
O	-2.36128439468247	2.43573600693971	-1.71422117702504

5⁰b (O-Si(CF₃)₄) E = -1713.288568 au

ZPE = 0.06199856 au

G = 0.01559792 au

Si	-2.92019919739716	1.14417379330865	-2.47670531597577
C	-3.70861418620926	-0.61964623613588	-2.44114979518675
F	-4.94350098007905	-0.59211045815304	-2.98462520607142
F	-2.97357839422175	-1.50531939137215	-3.14083058466413
F	-3.82435407929228	-1.08525293759606	-1.18250787189572
C	-4.20004960625977	2.43497553047213	-1.83609449531735
F	-5.23661944517001	2.55170138566294	-2.68973170766788
F	-3.63945139209325	3.65172384753199	-1.70217833614267
F	-4.69542686623214	2.07663679739043	-0.63439872792671
C	-2.43440185963517	1.54972079070499	-4.30002764717375
F	-3.48461768999444	1.34523195326635	-5.12098742233298
F	-2.04568507620205	2.83233541077323	-4.43888355735562
F	-1.42221311660057	0.76773746100745	-4.72462418276719
C	-0.38591753057228	0.78724245967681	-1.47438705750793
F	-0.35417198508400	-0.45504286968623	-1.98355943735433
F	0.09324923476484	0.75107128094792	-0.23753607488133
F	0.41019149981026	1.55953316956997	-2.22050875509099
O	-1.64788150953161	1.27633274263038	-1.45227854468721

5⁵a (S-SiF₄) E = -1085.954720640114 au

ZPE = 0.01311290 au

G = -0.01886552 au

Si	-2.18037762169266	0.90804704403688	-2.60636654091206
F	-2.32959989930611	0.98609630198953	-4.17164237879565
F	-3.79876168946006	3.22734382421099	-2.23229565672543
F	-3.26719177022031	-0.10974123804360	-2.09168849132685
F	-0.74496897421292	0.37328179232401	-2.23029673633245
S	-2.30743121510789	2.81836736548216	-1.68138540590753

5⁵b (S-Si(CF₃)₄) E = -2035.853582644874 au

ZPE = 0.05902773 au

G = 0.01239109 au

Si	-2.97671571660067	1.26243980179967	-2.44987543242930
C	-3.64330848971735	-0.55737631061713	-2.27040221830537
F	-4.95516059884177	-0.59502890951363	-2.58973998192702
F	-3.00729599829341	-1.41531468324266	-3.08938638039347
F	-3.51796522631117	-1.01790564327980	-1.01268023510690
C	-4.46845809874222	2.44853004374501	-2.08917321623821
F	-5.40048688244411	2.38060404303061	-3.05691933679887
F	-4.07091037037412	3.73403623584387	-1.99403681218276
F	-5.06266263276900	2.12296920202566	-0.92125653797707
C	-2.43376415383676	1.51279563111177	-4.29425805337582
F	-3.37524901196861	1.04658163461460	-5.13957506701878
F	-2.25025485352347	2.82090422260408	-4.56506040484916
F	-1.28240467637955	0.87360001549717	-4.57481603358271
C	-0.13371343470926	0.71674890124530	-1.42643129980520
F	-0.56911976138267	-0.45635355677649	-1.90982231028668
F	0.55518729388394	0.48450868910661	-0.30880231722619
F	0.69728360634312	1.24739725616174	-2.32435318897491
S	-1.51824317433273	1.86190815664353	-1.02442589352139

3^og E = -1798.039453276 au [PBEh-3c]

ZPE = 0.302081810 au

G = 0.25273339 au

O	-1.38107665270086	0.70044379526019	0.14350949672726
Si	-0.81494818734899	2.28539497719610	0.73880879395226
P	-1.97205409757424	0.23883615854774	-1.21207018109427
F	-1.91394107983716	3.19920729603316	1.50569622693994
F	-0.37627121566882	1.48433257463251	2.10003454580442
F	0.69524234608697	2.79373217248656	0.44296423470057
F	-1.31838399289052	2.89507673815019	-0.75266611062527
C	-3.37470723897104	1.20191039594530	-1.77276730416724
C	-3.64825538209496	1.32783266234052	-3.13066892189782
C	-4.22788348829676	1.76581108525144	-0.82768288232571
C	-4.78362203869068	2.00928544206109	-3.54290799282097
H	-2.97586443171098	0.90964550886388	-3.86921366368723
C	-5.35618901084720	2.44682556430459	-1.24819514513511
H	-4.01093985927190	1.69314295431971	0.22972436602545
C	-5.63585340143154	2.56681062086626	-2.60292245574574
H	-4.99404161525818	2.11258280749477	-4.59877406910614
H	-6.01240431740498	2.89651226598118	-0.51582199129973
H	-6.51735677087774	3.10466619086758	-2.92565596172156
C	-2.57346226966106	-1.42584926144388	-0.88825538049530

C	-3.56356459406993	-1.98936569321184	-1.68973205742537
C	-2.02460057839641	-2.15670153125547	0.16287661617507
C	-3.99240634275871	-3.28405981000132	-1.44945573937533
H	-4.01155099244241	-1.41820884169479	-2.49327159845254
C	-2.46206493463410	-3.45110433955619	0.39823301817310
H	-1.27139485710511	-1.71620670958259	0.80240803416592
C	-3.44020877135004	-4.01516648494838	-0.40692006685441
H	-4.76426172522170	-3.71859322798296	-2.07010290022867
H	-2.04028039746795	-4.01649824888870	1.21806834371362
H	-3.77990874446529	-5.02468677999353	-0.21694830686592
C	-0.75537724164422	0.13016629332376	-2.53222546716489
C	-0.41063265325803	-1.11489437831743	-3.05643678465641
C	-0.14077269558919	1.28536616256880	-3.02183880990241
C	0.53377672653581	-1.20482202326182	-4.06688161222689
H	-0.87137004160029	-2.01853690020397	-2.68102079150634
C	0.80072719879052	1.18304576998582	-4.03126981238696
H	-0.38864262550775	2.25366920132471	-2.61293611341026
C	1.13835209522003	-0.05718237466093	-4.55464001995120
H	0.79824585649212	-2.17383582255023	-4.46778358162340
H	1.27861084638788	2.07867343642996	-4.40400689378420
H	1.87741462653575	-0.12867543668179	-5.34167985044008

3^{oh} E = -3237.896531986 au [PBEh-3c]
 ZPE = 0.29665207 au
 G = 0.24498756 au

O	-1.62509255686998	0.83100510619416	0.11680690932540
Si	-0.46012754899088	1.96915359811236	0.76661590920878
P	-2.12709851077860	0.28008745978641	-1.24511319481941
Cl	-1.00038335461034	2.96617403409198	2.49979069968303
Cl	0.36358141066753	0.29054672246162	1.86051676609021
Cl	1.35360405916532	2.32733743448014	-0.19008788533494
Cl	-1.44406939970987	3.50697495397068	-0.47652272763560
C	-3.51607908572541	1.21257908206802	-1.87895442933679
C	-3.78052330198063	1.23899613677437	-3.24543839247030
C	-4.36972062851376	1.85204873511757	-0.98322766431180
C	-4.90612455658826	1.89889731861408	-3.71418647329951
H	-3.10773073124646	0.76091989393465	-3.94644700802361
C	-5.48919880370338	2.50971375244817	-1.46068845040335
H	-4.15266226348882	1.85745143924682	0.07622648518906
C	-5.75834356033592	2.53176286346715	-2.82265410069333
H	-5.10954215560872	1.92618711983142	-4.77602256302412
H	-6.14655795189198	3.01767844952550	-0.76861295022931
H	-6.63231308322046	3.05287448094622	-3.19020283851650
C	-2.67757744513737	-1.38839736970030	-0.88387608950662

C	-3.66529517206804	-1.98997630256021	-1.66015754690634
C	-2.07612164001200	-2.08794422256512	0.16130692139340
C	-4.04473843756085	-3.29556067416272	-1.39781937865829
H	-4.14953680967073	-1.44200581703411	-2.45864201680477
C	-2.46554666388945	-3.39410667886214	0.41517296586851
H	-1.31811186376585	-1.61952859872013	0.77816153780028
C	-3.44372051856465	-3.99691073703219	-0.36171722483851
H	-4.81541445852898	-3.76203144037807	-1.99623707538563
H	-2.00463501532588	-3.93801113182165	1.22836236815405
H	-3.74494725667310	-5.01536030319011	-0.15510504023058
C	-0.84762641194726	0.20418673456931	-2.49511037498461
C	-0.31326410996178	-1.02691931168839	-2.87151287969946
C	-0.36661012840595	1.38362164365722	-3.06727863169485
C	0.69471569413503	-1.07791614839796	-3.82025456851528
H	-0.67660166068201	-1.94463577307605	-2.42879579051215
C	0.64033112590394	1.31989762649579	-4.01383479321588
H	-0.75987717591698	2.34420826904997	-2.76078040370532
C	1.16950300529041	0.09343611966005	-4.39029261854047
H	1.11099559758640	-2.03309887422761	-4.10942726679178
H	1.02060308180932	2.23393690889214	-4.44844466213787
H	1.95993573681663	0.05130971002096	-5.12794431248559

6^N (Me3N) E = -174.163198741621 au [PBEh-3c]

ZPE = 0.12409799 au

G = 0.09687722 au

N	-0.37244419741933	0.65228022507270	-0.07591345956232
C	-0.04430684867782	1.41043927051311	-1.25662994465166
C	-0.05531278647754	1.37318874106736	1.13085714250719
C	0.22947951366373	-0.65691275476631	-0.09349843341634
H	-0.38085974475855	0.80482835354867	2.00350235583153
H	-0.58261043064386	2.32829518463954	1.14645001890837
H	1.02080446888269	1.58345644062020	1.25141529849403
H	1.03281857864135	1.62441300293964	-1.36051410904004
H	-0.57173126682902	2.36555769097620	-1.24735841533870
H	-0.36157015867054	0.86957146007292	-2.14955743816268
H	1.33236698143984	-0.63750321357386	-0.08798262198660
H	-0.09544211721148	-1.23053771860694	0.77592277252752
H	-0.08713629193947	-1.20308518250325	-0.98342182611030

6^P (Me3P) E = -460.426766838501 au [PBEh-3c]

ZPE = 0.11637512 au

G = 0.08723564 au

P	-0.84065194553321	0.58851025278922	-0.07905743243417
C	-0.07084412779114	1.53491744070151	-1.46916438739762
C	-0.08385690090384	1.49098132935492	1.34694836574469
C	0.25208720073431	-0.90358942477707	-0.09726031611865
H	-0.31023299194866	0.97057105655892	2.27758748114304
H	-0.51152571719763	2.49076986522780	1.42233651676988
H	1.00035826213810	1.58480932829540	1.25857128427123
H	1.01247018374534	1.62596664217396	-1.36780183650889
H	-0.49808224804889	2.53656801324215	-1.51739444587146
H	-0.28837529104802	1.04371714301239	-2.41761741861374
H	1.31370780603438	-0.64857100000449	-0.08837382700277
H	0.04043393573951	-1.52900309496717	0.77004851349133
H	0.04856753407975	-1.50165605160757	-0.98555115747287

H₂ E = -1.172386899707 au [PBEh-3c]
 ZPE = 0.01021926 au
 G = -0.00126753 au

H	-2.58606742470436	1.09848483000000	0.04264035000000
H	-3.32852583529564	1.09848483000000	0.04264035000000

7g^N E = -1973.364374947892 au [PBEh-3c]
 ZPE = 0.45089245 au
 G = 0.39501990 au

O	-1.20102615322715	1.15953336709980	0.05262186563420
Si	-1.31782981340026	1.78701070650545	1.61773504400875
P	-2.26346295142026	0.40928342206156	-0.92027423086160
C	-3.38643146021702	1.19151798576193	-2.17520879112876
C	-3.35123403770883	0.92125458045756	-3.54289636108615
C	-4.31933639864381	2.11122892748587	-1.70305077933992
C	-4.25418590596203	1.52680954150317	-4.40281797208816
H	-2.61926331772269	0.23549589008750	-3.94556066292898
C	-5.19845916060559	2.74776519228374	-2.56651841141043
H	-4.34367531224406	2.34397427790434	-0.64431546177173
C	-5.17452434563624	2.44608280073708	-3.91905473248208
H	-4.22777886616063	1.29053644834583	-5.45856139507712
H	-5.89888310821163	3.47826128179710	-2.18327436749331
H	-5.86469688414419	2.93151762546907	-4.59690818920745
C	-2.63448145915531	-1.37566030092268	-0.66910340266630
C	-3.85793908857252	-1.91538359359725	-1.05580987232596
C	-1.71257541034060	-2.18309518391481	-0.00940282315438
C	-4.14620210820175	-3.25179854669531	-0.81045564569991
H	-4.58208916388744	-1.29644402977767	-1.57391289582365

C	-2.00550941361749	-3.51581225361005	0.24417510938723
H	-0.75351666035650	-1.77731460079159	0.28635648415138
C	-3.21982972436630	-4.05525922703702	-0.15890163240107
H	-5.09035713590445	-3.66779196516340	-1.13835403011508
H	-1.27768670605005	-4.13746510606114	0.74964760505694
H	-3.43985977206461	-5.09877155582412	0.02562137808492
C	-0.84305220686329	0.14736126730227	-2.16188354570985
C	-0.68459441546606	-1.03238138884333	-2.88527498644746
C	0.01123981914353	1.21092632303666	-2.46298371063104
C	0.29404205458223	-1.15531898987071	-3.86555390261510
H	-1.32904663310778	-1.88201616893106	-2.69900870736390
C	0.98315812112782	1.09565115994006	-3.44355917029795
H	-0.07739609665932	2.14530142521843	-1.92433754316877
C	1.13194506678356	-0.09080136359374	-4.14898395516132
H	0.39703551501784	-2.08833724307709	-4.40526478457645
H	1.63249247779675	1.93597793363087	-3.65382571664652
H	1.89519916461506	-0.18235014753681	-4.91098862740356
H	-3.32543080144091	0.71058755503400	0.05360946322263
H	-3.13467875881836	-0.18248487909080	2.46337357502905
N	-4.06676835570971	-0.48850304775007	2.89617927568454
C	-5.17960679481666	0.10287645286124	2.12900398126964
C	-4.0947779223529	-1.96238427716474	2.84860668442596
C	-4.02624088074999	0.01990640450701	4.28134440187534
H	-6.12809035072315	-0.18920821935550	2.57809444416338
H	-5.07752588949587	1.18317914092138	2.13335322273685
H	-5.12877699195066	-0.24985177223314	1.10244166514699
H	-3.16316130553542	-0.40171831696580	4.78981856772608
H	-4.93695314833422	-0.26015005770018	4.80786974283636
H	-3.92317449551518	1.10029273335280	4.25603551133450
H	-3.20960780047620	-2.35292450737428	3.34352060100279
H	-4.09002456269240	-2.29015537548076	1.81246403833391
H	-4.98911903700950	-2.33168625072607	3.34847642127029
F	-2.76061848685879	2.25631768101790	2.26490634833480
F	-1.75496768397739	0.15296581245938	2.17909879755665
F	-0.02019731825213	1.67257741711390	2.57752281756375
F	-0.97866110455659	3.31338207519326	1.12736164124713

TS(3⁰g+6^N+H₂→7g^N) E = -1973.342225156093 au [PBEh-3c]

ZPE = 0.4439653240 au

v = -772.484890 cm⁻¹

O	1.54825574387792	0.60263553167209	0.83200119851344
Si	1.85686472402219	2.03992371966766	1.77131486653895
P	0.60595778995165	0.27480728864206	-0.38554374928651
C	-0.51248020022387	1.39311644082263	-1.29936919327771

C	-0.61822946884199	1.23914777087451	-2.68078905803142
C	-1.27259302566063	2.37001534723051	-0.66295157312888
C	-1.50608657120476	2.02104018396563	-3.40593027813111
H	-0.01265346710590	0.51166670194921	-3.20402109265434
C	-2.13019202346098	3.17174854140199	-1.39571614741147
H	-1.18513504466420	2.50641265724548	0.40456608701972
C	-2.25801371655626	2.99232136329041	-2.76607899694658
H	-1.59295509926290	1.87804187158646	-4.47470391918399
H	-2.69751545775831	3.94413911950746	-0.89397104710254
H	-2.93688026828764	3.61487921097040	-3.33415695668887
C	-0.02432548230634	-1.42153867092024	-0.27747396708313
C	-1.20921130439463	-1.80320604404519	-0.89831318699412
C	0.70663329664430	-2.35401492930006	0.45230629665822
C	-1.66363126278503	-3.10752547729643	-0.78164805615824
H	-1.78423952755048	-1.08087503313662	-1.46427626058611
C	0.24101711181686	-3.65609784039612	0.57352065519041
H	1.63648617346048	-2.06585805869678	0.92692709312992
C	-0.94350180025958	-4.03590268985032	-0.04117168033590
H	-2.58388048787892	-3.39977431097609	-1.27034087921923
H	0.81297622172108	-4.37734420252985	1.14268899610698
H	-1.30022720138627	-5.05346172096195	0.04862910866022
C	1.92099085069654	0.06900948904953	-1.66958959529272
C	2.06904453991191	-1.09456938870722	-2.41861196604245
C	2.78724541487671	1.13745148598339	-1.90946629308273
C	3.05995027508627	-1.19254666200740	-3.38756605967442
H	1.41493063736913	-1.94120267467418	-2.25752491333781
C	3.77346059999562	1.03735107459669	-2.87577529427490
H	2.68931967859732	2.05730293273283	-1.34902834068407
C	3.91431272440390	-0.12788602716797	-3.61747599260171
H	3.16224201089554	-2.10658262581610	-3.95790710204891
H	4.43827241762669	1.87369670643563	-3.04668283087789
H	4.68833102173584	-0.20361043650944	-4.37001236156409
H	-0.75318887067836	0.48541224278816	0.89828960802769
H	-1.03699094332948	0.12712647654109	1.85985241701569
N	-1.44508695071576	-0.29290986739532	2.93789846816566
C	-2.49322179998315	-1.25957087173694	2.61113645524926
C	-0.32535397298578	-0.90520457745793	3.66210514050176
C	-1.96753782854001	0.88580225454100	3.63413812061248
H	-2.96463965903008	-1.64697893080160	3.51637130613014
H	-3.24794526804352	-0.77709657286406	1.99251455015326
H	-2.06197937286214	-2.08452833690375	2.04682527306031
H	-1.16007148189869	1.59634028861026	3.78542775913976
H	-2.40201263263954	0.60718592624055	4.59570950625609
H	-2.73224845191671	1.35582291464970	3.01805938561772
H	0.49263544003451	-0.19474346890330	3.74211855595355

H	0.02436041131556	-1.77244158839296	3.10765832279402
H	-0.64339258646087	-1.22024125681660	4.65818877672103
F	0.62084169450572	2.69394487632020	2.63012278330715
F	2.24320990583520	1.03765249972026	3.03895460399024
F	3.33978265236609	2.69506806633340	1.77033915259820
F	1.41829989192574	2.95664928089520	0.43843230458996

7g^P E = -2259.609312460843 au [PBEh-3c]

ZPE = 0.43937644 au

G = 0.38225245 au

O	-1.55263564556840	0.48173146143032	0.39574643534598
Si	-1.41929988448425	1.88639531212062	1.34071892942830
P	-2.56674021681062	0.32799283805127	-0.92902027760346
F	-2.77291503044971	2.27364892593378	2.22769981268160
F	-0.89135638616009	0.94806837388424	2.63271644364011
F	-0.07710268518855	2.79293913125098	1.41030670029010
F	-2.01349881385562	2.82054882350179	0.06564129081090
C	-3.60099323384636	1.06644109361895	-2.31350485448005
C	-3.48673844909478	0.70756012518429	-3.65662752681561
C	-4.55901563096623	2.01027922034342	-1.96057899494614
C	-4.34370703044829	1.24190497686006	-4.60552291412806
H	-2.72946820029220	0.00238348030405	-3.97111404837987
C	-5.39955846504256	2.57175872293581	-2.91199696849803
H	-4.63467626152181	2.32537200902158	-0.92606587174822
C	-5.29950270995987	2.17949830459839	-4.23689055214547
H	-4.25586103525164	0.93550940095964	-5.63994397300927
H	-6.12470016201980	3.32004690175513	-2.61915077962139
H	-5.95529416162429	2.60899933946490	-4.98326515903335
C	-3.08525501003313	-1.42743043305421	-0.82084645273434
C	-4.34925351752654	-1.83237157309210	-1.24081848572505
C	-2.24195025947082	-2.36238449169357	-0.22190545936546
C	-4.76220185564154	-3.14705314616618	-1.07142144011901
H	-5.01200707462674	-1.11893041883074	-1.71585270825362
C	-2.65029811763545	-3.67989406070380	-0.06442860734028
H	-1.25478070906770	-2.06111477812873	0.10674889795395
C	-3.91219584525249	-4.07571305838443	-0.48647886518112
H	-5.74453080749704	-3.44898043628824	-1.41106261405575
H	-1.97715309616704	-4.39982910754938	0.38349625998712
H	-4.22807293322857	-5.10432367418194	-0.36934550402340
C	-1.03800253332980	0.20899572348542	-2.02672477103175
C	-0.70308291008192	-0.94717192063799	-2.72524051598085
C	-0.23955437843263	1.33966052462591	-2.20423038262283
C	0.40193910944193	-0.98105707093088	-3.56887398798196
H	-1.30456421466486	-1.84227661027490	-2.63036226323569

C	0.85810457178680	1.30797931492189	-3.04801173081669
H	-0.47636109434912	2.26147925566974	-1.69041723634778
C	1.18771470194896	0.14609298885745	-3.73277652455066
H	0.64268257125924	-1.89492529196922	-4.09741666610559
H	1.46267687671941	2.19780623991379	-3.16758200873293
H	2.04835543637002	0.12294693909456	-4.38857664483475
H	-3.64458829085257	0.77928136205564	-0.06324036451473
H	-2.63196631458963	-0.53511546900890	1.91413323835911
P	-3.64938689274515	-0.65265363339251	2.85921591500506
C	-5.14159079908218	0.16477822929825	2.27295476516477
C	-4.01526542476011	-2.41101454898285	3.04445107044001
C	-3.13075801954463	0.01617853438704	4.44506229607050
H	-5.94604871403055	0.02920979299747	2.99505159833999
H	-4.93853446688103	1.22394564558784	2.13718480325009
H	-5.43564388028292	-0.26382089516078	1.31608011735821
H	-2.18760865483702	-0.43762196291699	4.74122273336920
H	-3.89056997829329	-0.18790579177544	5.19764899825761
H	-2.97500221041494	1.08656406544445	4.34447814314016
H	-3.12781696382610	-2.94401153407469	3.38159828591601
H	-4.31603900022224	-2.82457136450732	2.08204973086059
H	-4.81481960757290	-2.56169876585286	3.76834839829392

TS (3⁰g+6^P+H₂→7g^P) E = -2259.592170069686 au [PBEh-3c]

ZPE = 0.4342786777 au

v = -854.549009 cm⁻¹

O	1.57644540167708	0.47708206421567	0.66293082507972
Si	1.91740698980570	1.83399080531762	1.69623853078509
P	0.55144861485790	0.29374702299471	-0.53120104027464
F	0.68906611185376	2.72444824987939	2.32341405358365
F	1.79892817278566	0.78578105345136	3.00488353494683
F	3.46773131046280	2.14715917986069	2.04337700940101
F	1.95257221570907	2.81879034192163	0.34974562403048
C	-0.26987570032429	1.58160919486992	-1.53804695126806
C	-0.34521187263336	1.42867271389584	-2.92213479794221
C	-0.85081065704297	2.69822827436277	-0.94368257174445
C	-1.02757928906328	2.35914700221923	-3.69145050826065
H	0.12494194195989	0.58634627260218	-3.41045652249418
C	-1.50197501842819	3.64221368592186	-1.71997266724399
H	-0.78727486211940	2.83408129199913	0.12634066084046
C	-1.60070860076444	3.47006237464309	-3.09293495222942
H	-1.09535642885676	2.21999339371640	-4.76220560036160
H	-1.92931755148937	4.51756600522134	-1.24966039390214
H	-2.11788164388171	4.20471534244619	-3.69632324174477
C	-0.42333761493850	-1.23303817829762	-0.38882450954148
C	-1.70478777138874	-1.33386083495570	-0.92376434229969

C	0.10709983446880	-2.29586962848752	0.33471185450251
C	-2.44037272126366	-2.49462850685348	-0.74932130210048
H	-2.12962426865041	-0.50307064648594	-1.47383301353639
C	-0.63828176800141	-3.45534561037877	0.51310876232430
H	1.10700061994270	-2.22730778681246	0.74570953812357
C	-1.90998515473061	-3.55828066946192	-0.02853442679645
H	-3.43080742364192	-2.57119676939265	-1.17852608449335
H	-0.21573367926913	-4.28332425223291	1.06807358300123
H	-2.48529284241037	-4.46521491205681	0.10327000847378
C	1.82287036816535	-0.24532035042217	-1.77167328464861
C	1.70195743273965	-1.41054021914179	-2.52212388737284
C	2.92564979997921	0.58218897658881	-1.99123936371128
C	2.66064260930225	-1.74792502190644	-3.47001070597887
H	0.85713536696483	-2.07179966775114	-2.37866269038333
C	3.87854582231517	0.24676324040860	-2.93793071829277
H	3.03919580094483	1.49902426482728	-1.42766555696052
C	3.75065955800836	-0.92054024263396	-3.67934243702390
H	2.55193992361418	-2.66093727908564	-4.04098736512153
H	4.72784756837588	0.89877535970463	-3.09452948775056
H	4.49912376614859	-1.18190298364463	-4.41604619132641
H	-0.63975986998585	0.79490608388601	0.65417387610746
H	-0.80177804833785	0.37738447403241	1.61670311511388
P	-1.08269811660155	-0.24180632133945	3.09277597444105
C	-2.76208661165483	-0.94670598097905	3.02455491998201
C	-0.04720195023463	-1.56045179880035	3.79492951920499
C	-1.14932641969592	1.07787069779065	4.33618468209284
H	-3.08639903028348	-1.32277376366475	3.99475882275695
H	-3.46819249233144	-0.18779755258510	2.68968881520017
H	-2.77972093240976	-1.76362497508725	2.30256531588929
H	-0.14282611857922	1.44564081450543	4.51574972673512
H	-1.57960885737218	0.70934527246583	5.26701776937150
H	-1.75082638611322	1.90606059228713	3.96629241420228
H	0.99194286281627	-1.24502885036940	3.77245900634710
H	-0.16111270308305	-2.46861257607976	3.20726557078050
H	-0.34439968731649	-1.76468866712909	4.82416110148679

7h^N E = -3413.228469327662 au [PBEh-3c]

ZPE = 0.44572514 au

G = 0.38739326 au

O	-1.05586148901893	1.01747481314468	-0.02960481053493
Si	-1.07683800039644	2.05718149119518	1.27241323020457
P	-2.26577252683768	0.43653567059389	-0.99667347364555
Cl	-2.79791236618442	2.69852421164133	2.33414306308411
Cl	-1.23485115815234	0.05541056290906	2.59971970824059

Cl	0.72603822474741	2.43058185176891	2.17839934193890
Cl	-1.11863948748527	3.80931426742312	0.04631034188212
C	-3.46767561153580	1.25574631751150	-2.14564912794542
C	-3.56589722934108	0.95777958755192	-3.50481235214786
C	-4.32022884381934	2.21490088717438	-1.60645651978423
C	-4.52915137451486	1.57205549810385	-4.28887309031520
H	-2.89313900660376	0.24176580424308	-3.95671655003211
C	-5.26005190709930	2.85821187586734	-2.39860259573791
H	-4.23182781006658	2.47828744239822	-0.55854635421986
C	-5.37336484275700	2.52775543676548	-3.73958876446858
H	-4.60955019858354	1.31569172312010	-5.33711958110018
H	-5.89665402295735	3.62074403558767	-1.96950633857441
H	-6.11019418123784	3.02099537573050	-4.36023313909991
C	-2.69029339890571	-1.33093854676243	-0.75521923174740
C	-3.90537995711319	-1.85380907523407	-1.18923552984166
C	-1.79100677356550	-2.15625663269798	-0.08396428504610
C	-4.21209466969111	-3.19098157835598	-0.96971579358865
H	-4.60710908011013	-1.22455719612085	-1.72445313445038
C	-2.10053327141430	-3.49155203913899	0.13293799641742
H	-0.84550289017764	-1.76021780771550	0.26241474749124
C	-3.30833024038806	-4.01343183877965	-0.31107117697531
H	-5.15121340190613	-3.59263527510805	-1.32817851808980
H	-1.39036474566511	-4.12732120903476	0.64555947271822
H	-3.54095901930869	-5.05831019960912	-0.15143727542144
C	-0.94977798182777	0.19327079935474	-2.33772020879037
C	-0.77279374058516	-1.00457891725444	-3.02280828442981
C	-0.19456505386112	1.29718848525930	-2.73925506464032
C	0.13424566819133	-1.10393703110008	-4.07301183858714
H	-1.34168791113745	-1.88445310640148	-2.75245828920072
C	0.70417469055258	1.20267315415753	-3.78810304057068
H	-0.30666306076417	2.24732125644871	-2.23103494806345
C	0.87493418805676	-0.00115203165260	-4.45963424767602
H	0.25795770890408	-2.04991234940048	-4.58488530638186
H	1.27875838731550	2.07250776505872	-4.07945226386673
H	1.58135340239327	-0.07579077604849	-5.27623850540613
H	-3.19815489957593	0.79773847618455	0.07851749320348
H	-3.25096729259164	-0.15924293045738	2.44750322172045
N	-4.19225712815611	-0.48266717436022	2.78912050601909
C	-5.26006973863224	0.07908266115883	1.93900106437389
C	-4.14763343236407	-1.95787851885090	2.72340699889334
C	-4.27126678313878	-0.00000816098746	4.18381979229185
H	-6.22832424462199	-0.25427080390035	2.30876700746845
H	-5.20001865640736	1.16263828592031	1.96422424637608
H	-5.11487865217648	-0.25986611108416	0.91699284453230
H	-3.41003814806964	-0.37397768669800	4.73011004655572

H	-5.19377416904667	-0.35241024858988	4.64051156097673
H	-4.23629914541966	1.08489415689143	4.18391477419379
H	-3.25706362276665	-2.30173921744290	3.24226413301356
H	-4.09329515032476	-2.27118898595722	1.68492754688772
H	-5.03951448384965	-2.37107987442072	3.19061907189773

TS (3⁰h+6^N+H₂→7h^N) E = -3413.199152225014 au [PBEh-3c]

ZPE = 0.43811424 au

v = -893.67 cm⁻¹

O	-1.11906643313020	0.79828410326653	0.07057804709062
Si	-0.86735165701621	2.09059111529308	1.17450037338488
P	-2.16301323343548	0.28633061054199	-0.98651736766101
Cl	-2.23757407879236	3.19166941535543	2.31654919010983
Cl	-0.78143378410114	0.53929864485958	2.74794432520097
Cl	1.14163179082016	2.54622010226481	1.39528885303772
Cl	-1.13222577923995	3.47647530874143	-0.49262795154837
C	-3.43097560771669	1.27864961544212	-1.84574415811934
C	-3.04748314153272	2.06292420523097	-2.93278294651437
C	-4.77429946781251	1.24023186757103	-1.48443997003424
C	-3.99393950880959	2.78571866207047	-3.64072069053386
H	-2.00997895357853	2.12815892236961	-3.22487935591124
C	-5.72369573005446	1.93210058082571	-2.21641181665067
H	-5.07203468383291	0.67763249124731	-0.61164201484593
C	-5.33347104435678	2.71373561619040	-3.29367186850302
H	-3.67761728534590	3.40809180795489	-4.46657578845231
H	-6.76589228113542	1.87883755742534	-1.93091460948088
H	-6.07078795792443	3.27309286967816	-3.85426834032050
C	-2.61458688211477	-1.44066951674647	-0.68044397861139
C	-3.76902996743889	-2.02137065217161	-1.19640543528548
C	-1.72658162006116	-2.20748094022523	0.06920573039154
C	-4.03885952167571	-3.36030538210788	-0.95294762401150
H	-4.45871415035723	-1.43829923919444	-1.79393563696984
C	-2.00231993532440	-3.54562682449691	0.30404920996301
H	-0.83257789501647	-1.76163817931638	0.48580785105566
C	-3.15747034500251	-4.12498299866852	-0.20166904913960
H	-4.93535783816109	-3.80847331514516	-1.36121593962509
H	-1.30918999767608	-4.13672041168075	0.88784962223077
H	-3.36673475602358	-5.17043252518012	-0.01762887305243
C	-0.98218561473364	0.02583660253252	-2.38049697814892
C	-1.36184950091337	-0.78691202054628	-3.44803619074248
C	0.26756188840995	0.63779705973296	-2.41104952359761
C	-0.51348360376683	-0.98677373692184	-4.52327900093024
H	-2.32797748140631	-1.27678276391355	-3.44820699887297
C	1.11720928457352	0.43626933324698	-3.49111768097900

H	0.58807052757171	1.28319996760321	-1.60604380445180
C	0.73172590478543	-0.37361223844385	-4.54634819517011
H	-0.82274617484741	-1.62330409710212	-5.34176056325619
H	2.08530841240066	0.91915380108740	-3.50172622457797
H	1.39822929758033	-0.52909462070241	-5.38458496943969
H	-3.37816069947280	0.51630772227412	0.50562289503297
H	-3.83572855230517	0.17249460288298	1.40273117942506
N	-4.46130455740952	-0.27081661187760	2.38432772561497
C	-5.83066059259261	-0.46817313749835	1.91350101345073
C	-3.83014627238129	-1.53510514873009	2.77394027749106
C	-4.38886099747092	0.72589837652639	3.45770651443264
H	-6.46340602131032	-0.87665597895108	2.70397608687566
H	-6.24426879886450	0.48572201553545	1.59005456746306
H	-5.82656069947894	-1.15773390898977	1.07042156198781
H	-3.35141844225109	0.86136044907756	3.74984888305035
H	-4.98016890140809	0.40059153123029	4.31659385591488
H	-4.76720531314160	1.67809225375107	3.09425028110012
H	-2.78072053629890	-1.34922360824287	2.98725083626368
H	-3.90274073559873	-2.24658208403892	1.95435065191533
H	-4.31985860381639	-1.95189070091747	3.65708258295585

7h^P E = -3699.483082237902 au [PBEh-3c]

ZPE = 0.43346387 au

G = 0.37425041 au

O	-1.85471216557214	0.28382052347414	0.47450745682505
Si	-0.67363090279168	1.10107785610149	1.27299536589768
P	-2.74203244509493	0.48672055522637	-1.05121041030935
Cl	-1.02363782292397	1.56759379101651	3.32715132641264
Cl	0.06620355698086	-0.95698445753452	1.97435154284212
Cl	1.21717290383835	1.55828167839484	0.57437263627893
Cl	-1.48458944241306	3.06457430855908	0.69728656231903
C	-3.77316349097882	0.81041214260133	-2.61628165872283
C	-3.60763566846882	0.07913864456352	-3.79286948567047
C	-4.72070090837868	1.82471582998635	-2.60297597566440
C	-4.37689425725885	0.34657638440388	-4.91144760457289
H	-2.86416754865001	-0.70918438113631	-3.83587877566052
C	-5.49595584060739	2.10585120333291	-3.72405753303907
H	-4.85666009904906	2.42063191216771	-1.70456337735618
C	-5.32633113708380	1.36306545771964	-4.87934264801852
H	-4.23541932569579	-0.23151218628238	-5.81571151467742
H	-6.22479272349713	2.90571688228258	-3.69316208917725
H	-5.92393063255109	1.57601898497896	-5.75618238239640
C	-3.42179889893494	-1.21210539381763	-0.79315526289813
C	-4.73333765485007	-1.50571881731953	-1.16539271280691

C	-2.63957960360283	-2.23581483678340	-0.25088475703359
C	-5.24966135358616	-2.78478576590717	-1.00864122090868
H	-5.36241912370051	-0.73900787480355	-1.59661853968917
C	-3.14088929608555	-3.52584312959553	-0.14807599526966
H	-1.63950845853733	-2.03460478898423	0.10839002858958
C	-4.44730196718412	-3.80588207317880	-0.52241185573047
H	-6.27373360184229	-2.98512047521377	-1.29513176185341
H	-2.50434239244490	-4.31151023789766	0.23804803574198
H	-4.83775551036834	-4.81153645878953	-0.43431702292300
C	-1.16849789259555	0.67996563336428	-1.95857033121412
C	-0.19563999001601	-0.31286636246851	-1.95389102538939
C	-0.93718618920916	1.86437766721923	-2.65036548743691
C	0.98400667745253	-0.13274489339356	-2.65898373060673
H	-0.33436936536738	-1.22739319397290	-1.39512360789663
C	0.25986037978767	2.05608533956965	-3.31882090812506
H	-1.68511160943638	2.64598716182616	-2.66163834843464
C	1.21832522686077	1.05377226950017	-3.33399486368651
H	1.73175377756137	-0.91437571520571	-2.65481413403579
H	0.44231948686701	2.99161828040121	-3.83033751510351
H	2.15001315661589	1.20195976362692	-3.86388361988886
H	-3.41639745198194	1.56380691118353	-0.44181017814892
H	-2.18273553636819	-1.05847319051631	2.55541945587010
P	-3.44157401790517	-0.81221200095881	3.13401707622469
C	-4.30187094280640	0.61586855434547	2.45355540925995
C	-4.50031856168419	-2.25426660991539	2.88148148755285
C	-3.22847316773905	-0.62369292148512	4.91633645910837
H	-5.20445693507322	0.79069840025229	3.03912515636190
H	-3.67000859209048	1.50083834950363	2.47850381745544
H	-4.58193139013349	0.40676632960883	1.42374467752189
H	-2.70114166624089	-1.49000785673072	5.31275409153712
H	-4.19757255044029	-0.54136860980432	5.40598686410828
H	-2.63648482600074	0.26391974453012	5.12322061784074
H	-4.00373807456662	-3.15166393905195	3.24677650852872
H	-4.71684878425062	-2.39141270241878	1.82337140060577
H	-5.43720965990492	-2.12564466657463	3.42241006746284

TS (3⁰h+6^P+H₂→⁰h^P) E = -3699.458714979 au [PBEh-3c]

ZPE = 0.433332290 au

v = -37.74 cm⁻¹

O	0.76903532041650	0.58565790389059	0.99320931810403
Si	2.04699654871658	1.57541657695106	1.51156504216132
P	0.09158080137011	0.04721078286712	-0.43968156091106
Cl	1.80500667340957	2.21000674909671	3.51457244992994
Cl	3.10479960676272	-0.24429359941629	2.19819184186450

Cl	3.77308760829904	2.31202193947069	0.64165772525120
Cl	0.86525665533470	3.31495068883546	0.77636057247574
C	-1.01207206666594	0.63010223423446	-1.82668842767248
C	-0.74356431430491	0.38937386378056	-3.17461652170931
C	-2.17308584608760	1.31477468282869	-1.49287347153573
C	-1.63904437133088	0.79191882134037	-4.15207849055387
H	0.16587186327304	-0.12190484890857	-3.46339055866494
C	-3.05456744179839	1.75486135391081	-2.47005444387291
H	-2.38778156451763	1.51604794709760	-0.44944501241151
C	-2.79163566445208	1.48407780006295	-3.80271813121297
H	-1.43045576441455	0.57729300620307	-5.19193713369755
H	-3.94217947086193	2.30739174487967	-2.19083710345830
H	-3.47888333682529	1.81587595949247	-4.56994229306523
C	0.10194542745827	-1.78582090353307	-0.45791891847709
C	-0.59652458374152	-2.51823296498086	-1.41341136979857
C	0.76104761544732	-2.46642943312370	0.56520200921312
C	-0.62899075744589	-3.90405865134792	-1.35246959823064
H	-1.12264524359383	-2.01562015609796	-2.21356785176254
C	0.72837701902919	-3.85263724680224	0.61951538306967
H	1.33535504707192	-1.92223015987006	1.30448657760635
C	0.03325993007483	-4.57652996501707	-0.33707672307179
H	-1.17118717778368	-4.45818555692608	-2.10759602037102
H	1.26184780277046	-4.36622539458927	1.40911149346344
H	0.01356522520803	-5.65780464610456	-0.29616018040439
C	1.67539773766699	0.41768823152335	-1.38313670152717
C	2.73318754165731	-0.48800078802780	-1.40540865326461
C	1.82613604176263	1.62986428949438	-2.05628022364098
C	3.90089506221419	-0.19834712282696	-2.09591563817649
H	2.66042795611839	-1.43357371209231	-0.88657318508380
C	2.99332449115763	1.92094559674506	-2.74252826799015
H	1.03376711555648	2.36601846800428	-2.03955494765460
C	4.03377129950069	1.00537924159722	-2.76796739909419
H	4.71059530825174	-0.91626621541117	-2.09926697980004
H	3.09249606397207	2.87258765463267	-3.24778114925908
H	4.94746903994603	1.23316190172401	-3.30148350600580
H	-1.14179668824589	0.04922910176151	0.35394543673712
H	-1.78070566035941	0.05183360497555	1.86758120987469
P	-1.62284193159115	0.39383997308141	3.22139320230840
C	-1.49768623629186	2.18528235599220	3.31288638368754
C	-3.13766260019161	-0.09462264712123	4.08685958032088
C	-0.27709302413841	-0.54963542433986	3.94713265777378
H	-1.13762976553237	2.49759907507655	4.29040753288804
H	-0.81571876741377	2.56793945596537	2.55158726957036
H	-2.49051315916861	2.60202166658121	3.14270814893925
H	-0.53847645318599	-1.60575052483706	3.88589504505731

H	-0.16064231866758	-0.26784437968738	4.99246623005958
H	0.66778743435420	-0.39239529364117	3.43325411135572
H	-3.27714520938581	-1.17302427589246	4.03396243800688
H	-4.00407092473757	0.39032903032897	3.64003360468458
H	-3.07768789406652	0.19873220816900	5.13437519797538

3^oi E = -3284.946037504656 au [PBEh-3c]
 ZPE = 0.17713930 au
 G = -3283.03827118 au

O	-1.33203483004524	0.72516049988097	-0.01572857149772
Si	-0.46474662964489	2.50689495572301	0.53541349435909
P	-1.96299647186579	0.14500654675444	-1.24762681119209
F	0.21694591306672	3.90974387585145	0.96121093764811
F	-0.53826552708115	1.83087883047411	1.98286658793620
F	0.68813817259248	2.02134971974378	-0.48345617097866
F	-1.81377117471846	3.12725368431452	-0.09986314555893
C	-3.42741105348407	1.06680948376997	-1.79100607321970
C	-3.74155072883218	1.42335544226438	-3.09594834866492
C	-4.30468066416141	1.46418852946713	-0.78634182665670
C	-4.86050209985727	2.17898530388320	-3.38830423455423
C	-5.42992578582954	2.21684866948671	-1.05720943527430
C	-5.70103606562707	2.58093944876368	-2.36470771242689
C	-2.60923111549313	-1.50719421115991	-0.90701666108487
C	-3.35640104809563	-2.15947259615443	-1.88013140914749
C	-2.43498780254100	-2.14658365012396	0.31539649013876
C	-3.93404878332410	-3.39020798541972	-1.66391156495976
C	-3.00892507064750	-3.38681296386012	0.55228248415307
C	-3.75710810354541	-4.00354691472627	-0.43284996294350
C	-0.76939852931223	0.04835342147330	-2.60040605804265
C	-0.11686744020991	-1.11996634328911	-2.97034579628665
C	-0.32740444016829	1.23777418146818	-3.16981407758880
C	0.90759726044276	-1.11215465001575	-3.89866210113667
C	0.69102754634361	1.27090567718797	-4.09756974558937
C	1.31006547993018	0.08575705028768	-4.46099362104556
F	-3.50348185749039	-1.58639439626827	-3.06994167238560
F	-4.63899181977610	-3.98710600806189	-2.60990724358546
F	-4.29935851919379	-5.18199666402562	-0.20657757608504
F	-2.84012638082337	-3.98460590341323	1.71845811454126
F	-1.72194433657895	-1.61441325572482	1.28209811289188
F	-0.44568289124582	-2.28714724411804	-2.43439411555128
F	1.50731589491077	-2.23956525907004	-4.24233647374409
F	2.28504596421778	0.09983325587989	-5.34528554040532
F	1.07882968829257	2.41199707510154	-4.63648278511191
F	-0.91130504862759	2.37615457150048	-2.83405477091558

F	-4.09081129333436	1.08540284008821	0.46128946970749
F	-2.98471206808303	1.03831784380802	-4.11259344760743
F	-5.13670872279046	2.51092091419790	-4.63846728561342
F	-6.77167074588182	3.29692170118283	-2.63891992449887
F	-6.24862200148632	2.57929887287788	-0.08557880802202

3^{0j} E = -4724.790107872177 au [PBEh-3c]
 ZPE = 0.17219103 au
 G = -4723.17626229 au

O	-1.63073256344538	1.32811051919139	-0.21929281901337
Si	-0.10766140337627	1.61622356414079	0.66360552864125
P	-2.05364898902584	0.35358242850497	-1.33870375564584
Cl	0.19883754573137	1.16652604558042	2.65570527981637
Cl	0.36973535056559	-0.52545299068774	0.13790213501017
Cl	1.46971274215637	2.26342974798194	-0.52089489686035
Cl	-0.86985990443878	3.55125459684355	1.05562904749464
C	-3.55688113776042	1.09926770250226	-2.02299559132837
C	-3.81705161849677	1.31561944058946	-3.37069354044828
C	-4.53975210227058	1.47277649319971	-1.10943420366048
C	-4.99156023781969	1.91229930648034	-3.79033970744685
C	-5.71921156638189	2.06815268577530	-1.50856026084867
C	-5.93933972361711	2.29377273762053	-2.85710818773146
C	-2.64606370494078	-1.24270295983575	-0.76534236406512
C	-3.16699298973139	-2.11873562810816	-1.70871879113054
C	-2.71009234879384	-1.60525390357324	0.57529566605447
C	-3.68922856515352	-3.34379331442020	-1.36051242227751
C	-3.23421093719455	-2.83282341929139	0.94505676663540
C	-3.71608989351803	-3.69919434342755	-0.02031149742127
C	-0.80513412283478	0.26061300985376	-2.62096234171495
C	-0.11851117622935	-0.88938657534085	-2.98971025944574
C	-0.40095192829713	1.47058432439482	-3.17379569544773
C	0.91935257844441	-0.83477326460106	-3.89720918334104
C	0.63724079360995	1.54655596412578	-4.07687267100272
C	1.29660404991731	0.38399671890850	-4.43750691259808
F	-3.15848856021313	-1.75795340683148	-2.98839395601476
F	-4.16542994533814	-4.16618172831105	-2.27895408667976
F	-4.21592149708983	-4.86376721852820	0.33468661770020
F	-3.28924265163948	-3.17511674580697	2.21865747271014
F	-2.31047839921291	-0.79574028203929	1.52847697145284
F	-0.42695568781983	-2.06210889281059	-2.47051723076277
F	1.56179343529333	-1.93590646891724	-4.24533213021529
F	2.28771289838409	0.43520458837259	-5.30118662188241
F	1.00142650947606	2.70602702417320	-4.59199181686458
F	-1.03253715550934	2.58111574327803	-2.82666092576383

F	-4.36566150039481	1.22468753236973	0.17723760795728
F	-2.95554009288409	0.94808228032452	-4.30532097249089
F	-5.21433652213373	2.11342679802955	-5.07727317359817
F	-7.05947862036609	2.85890873391798	-3.25351195615579
F	-6.63511348765070	2.41055750637164	-0.62156240161595

TS ($3^{\circ}\text{i}+6^{\text{N}}\rightarrow 7^{\text{iN}}$) E = -3460.230098118337 au [PBEh-3c]

ZPE = 0.31903872 au

G = -3458.10059796 au

P	0.04492137051408	0.27490234216078	1.14635863726803
C	-1.36187976329945	-0.88930576786800	1.32065663173058
C	-2.44218280365400	-0.52691746739114	2.11485392557818
C	-1.40106592232827	-2.16443094762499	0.77552596566357
C	-3.52094062681865	-1.36896041521568	2.32663965248135
C	-2.46034150417061	-3.02577578043312	0.97688881312315
C	-3.52836644666443	-2.62846792831343	1.76063728603752
C	1.58651916552334	-0.30966869177485	0.36544591552822
C	2.15660700322124	-1.48786881652325	0.82615792502507
C	2.32899964928933	0.46076174579795	-0.51523437469723
C	3.38292183229275	-1.92939376829939	0.36357962230278
C	3.56412076182912	0.04937658352954	-0.97196202618164
C	4.09083959010246	-1.15401626844418	-0.53328105962318
C	-0.55010810088767	2.00369826515151	0.85914223412786
C	-0.71550188914277	2.84334399277601	1.97695430698393
C	-0.83074377227225	2.61414321849368	-0.36898713632073
C	-1.11623462494658	4.16447687013658	1.87243650720715
C	-1.22809387396124	3.93394408521828	-0.48295980397244
C	-1.36994838581054	4.72123185067365	0.63839696865266
F	1.53505960568231	-2.22881791316477	1.72793648602123
F	3.88642217028845	-3.07548616788231	0.79083264697169
F	5.26696723656335	-1.55826372984995	-0.97740310374077
F	4.24881924667550	0.80046729927629	-1.82382680424566
F	1.86512050516067	1.62076854617563	-0.95741166571239
F	-0.54931476967000	2.43919160063209	3.21701899978447
F	-1.26491500588932	4.89359687979875	2.96462007104077
F	-1.75181216729265	5.97733194814920	0.53101158262637
F	-1.47287084852058	4.44288723823153	-1.68361037157718
F	-0.73792852224190	1.99737801475667	-1.53730363990133
F	-2.49492876272495	0.66966341799555	2.67594993467983
F	-4.53987990459330	-0.97106192681358	3.06960430971080
F	-4.54859512016736	-3.44275046971688	1.95452491995638
F	-2.45720222590850	-4.22620340947095	0.41368520072655
F	-0.41639435671915	-2.60588264720349	-0.00246229314901
O	0.49433112295710	0.23235679135883	2.64908158125348

Si	1.98233523296594	0.90324007352139	3.37318592919841
H	-0.52172736272661	-0.08193794239421	-0.67332263313054
H	-0.39874484443487	-0.47206344186249	-1.60837884603531
N	-0.31489915961775	-0.97166421296440	-2.81276418777133
C	0.80329704187765	-1.91725808667553	-2.88029729085607
C	-0.11594835430939	0.12895695681698	-3.76072289194931
C	-1.60174053380335	-1.63631247891401	-3.03067769975673
H	0.88214942825208	-2.34988445344235	-3.88047081453750
H	1.73273066302548	-1.40112251659692	-2.65084659612409
H	0.66313116178642	-2.71859681234262	-2.16244426284431
H	0.78036780747223	0.68472388870379	-3.49548582627975
H	-0.96650921994571	0.80390848408396	-3.73284507264433
H	-0.00739718865548	-0.25743977937572	-4.77661203578659
H	-1.67552356679017	-2.02909903603363	-4.04697152579875
H	-2.40747787616476	-0.92316322593847	-2.86636882129216
F	1.66992745806324	-0.06351799298782	4.65664203182162
F	3.32524115952479	0.10351048621950	2.91531421637061
F	2.13986043505652	2.22084545265228	4.30428042632000
F	2.05379140500221	1.88873085595647	1.99318762305937
H	-1.71526354899396	-2.45810479274873	-2.32789956732328

TS (3^oj+6^N→7j^N) E = -4900.087892700379 au [PBEh-3c]

ZPE = 0.31359282 au

G = -4898.24865333 au

P	0.06238825463759	0.33318309194054	1.11257626168424
C	-1.30459542611167	-0.86405159448392	1.35114373863667
C	-2.35380280070123	-0.52597710371972	2.19767480087326
C	-1.33681745280906	-2.14359109138090	0.81371801956338
C	-3.39375767661829	-1.39699220222328	2.47271605053264
C	-2.35702952317153	-3.03419184283474	1.08057341461787
C	-3.39263326563155	-2.66150008087714	1.91777567867548
C	1.59220167780208	-0.26288993076976	0.32679957181840
C	2.15232596989871	-1.44596991801682	0.78667865240408
C	2.30876887429659	0.47123451271217	-0.60619018370043
C	3.34859540457864	-1.92486710130884	0.28215695198583
C	3.51234333254087	0.02146176914361	-1.10579007714971
C	4.03131391650177	-1.18540370251695	-0.66302021590769
C	-0.58088692570365	2.03582597284872	0.80069745608348
C	-0.77705598573698	2.89060553335423	1.90287946765361
C	-0.88500632740372	2.61069248464231	-0.43950125991247
C	-1.22943709593007	4.19195376114920	1.77282111705627
C	-1.33284206091168	3.91156783997145	-0.57818939102349
C	-1.50572318476833	4.71392054310676	0.52819382636077
F	1.55211025422217	-2.14763825419565	1.73226274061903

F	3.84936436017404	-3.06648769085855	0.72048388048386
F	5.17971611674362	-1.62224074244661	-1.14503356622301
F	4.17385574399581	0.73686310860217	-2.00410511055552
F	1.84967437004629	1.63097868278253	-1.04870811287082
F	-0.57714951937997	2.52197854056533	3.14732526461951
F	-1.40005270632510	4.93690781418354	2.85034114516339
F	-1.93589483652536	5.95121736432743	0.39680935808202
F	-1.59775720173219	4.38654306704235	-1.78794682380958
F	-0.76635355701450	1.97511465276754	-1.59480347953533
F	-2.41406833794936	0.67367204275803	2.74862976896136
F	-4.38359820830551	-1.02165004542116	3.26392122430952
F	-4.37486657201101	-3.50361372821058	2.17278156988208
F	-2.34635212157841	-4.24026296548342	0.53139875497048
F	-0.38159577548017	-2.56565827933799	-0.00827739256747
O	0.53864963586280	0.34649427648482	2.61494597150071
Si	1.91128071320176	0.80045984593792	3.59665941324210
H	-0.51842188806043	-0.08125523583285	-0.70091206181642
H	-0.39601325480546	-0.45805335129797	-1.61348416246118
N	-0.30251453941495	-0.95520988374131	-2.85753552675035
C	0.67310195007146	-2.04772975306009	-2.88846047517281
C	0.10147239812909	0.11244575994291	-3.77677313746906
C	-1.65606120223123	-1.42815164162663	-3.14890627423660
H	0.79401156328709	-2.42828352041930	-3.90577390718953
H	1.63768010671739	-1.68735992314600	-2.53634359706793
H	0.35082159540912	-2.86322516564630	-2.25012982389995
H	1.04931437118966	0.53887267257653	-3.45686657969185
H	-0.64607402328548	0.89960836410917	-3.79298264694189
H	0.21629928432883	-0.27982276199022	-4.79018663755183
H	-1.73037409325937	-1.82446745110325	-4.16423344103513
H	-2.35827427577470	-0.60389826491075	-3.03804819950735
Cl	1.24389139994384	-0.68959469354560	4.97542127871122
Cl	3.73411974310570	-0.14310331218365	3.21943406769149
Cl	1.93390645195927	2.30048011073507	5.02591459907300
Cl	2.36619835488249	2.32301002135415	2.00439659395791
H	-1.92839600489563	-2.21195060044849	-2.44492855516624

7i^N E = -3460.255137966063 au [PBEh-3c]

ZPE = 0.32733322 au

G = -3458.11176275 au

P	-0.16319078397723	0.26685345069742	1.00482614110432
C	-1.47985027285917	-0.93204592693060	1.51131378627908
C	-2.33388621599421	-0.69564382547163	2.57941702151750
C	-1.65839041923734	-2.12753892359716	0.83716419620454
C	-3.31442829165830	-1.60339911208056	2.94793367519493

C	-2.61216168599628	-3.05964917148592	1.18933788841143
C	-3.44808526674294	-2.79348389342800	2.25818510546461
C	1.43746854793953	-0.43556981922273	0.32422822357998
C	1.95821802028244	-1.63227018333112	0.78576801712557
C	2.21894943840228	0.30516437803901	-0.54105888580465
C	3.19317500454017	-2.09695069645966	0.37054568492464
C	3.46352190695507	-0.12338443089488	-0.95955961829748
C	3.95333055543800	-1.33205156894854	-0.49564999865036
C	-0.77112378250443	2.02905896615145	0.85115193238316
C	-0.88299775330757	2.91181566920537	1.93293840557111
C	-1.11863122059580	2.57728160615314	-0.38561091526304
C	-1.30934849459880	4.22315267319039	1.78340046460872
C	-1.53498985997485	3.88184080945095	-0.55715780310479
C	-1.63035168440447	4.71659279919114	0.53687584483793
F	1.27406785640053	-2.37354786493128	1.64377766857422
F	3.65848187654330	-3.25982563397080	0.80048742996189
F	5.13704399235824	-1.76360269806400	-0.89946803514622
F	4.17897651016755	0.60461969702705	-1.81172514827241
F	1.76292295346090	1.46003426917394	-1.03334723328047
F	-0.63262778092404	2.56242677122496	3.17367035225254
F	-1.41471595672554	5.00928198261589	2.84183769259942
F	-2.03323321137658	5.96489696884751	0.38975719962110
F	-1.84199981622356	4.33179513939432	-1.76991315248779
F	-1.07206150735444	1.87304285488545	-1.52919797663944
F	-2.27882438943716	0.43474388331828	3.25645122533194
F	-4.12882229502216	-1.33563784022499	3.95601347612714
F	-4.37655816826934	-3.66685555592314	2.60666517202446
F	-2.73073530608421	-4.19522445607619	0.51078430952979
F	-0.87906197499203	-2.43103846727463	-0.21406344456340
O	0.45082089744997	0.33870549642059	2.48919120777627
Si	1.96068183142350	1.01333063777697	3.05962368540344
H	-0.68608034198975	0.07538879355989	-0.35577074506857
H	0.01930474183474	-0.47141393920237	-1.90820494604775
N	0.04707885939156	-0.81820800507651	-2.88024755562765
C	0.84965561846238	-2.06716577753520	-2.89419927686392
C	0.67050990720420	0.22637836939493	-3.73356432091982
C	-1.36517382925222	-1.06204352328012	-3.26511005150480
H	0.92389595340909	-2.42639364368321	-3.91800053268986
H	1.84198057994188	-1.85579216993511	-2.50567450326369
H	0.37229217438527	-2.81768547604308	-2.27431050205416
H	1.70193243506772	0.37893524245391	-3.43208149195892
H	0.12382891309727	1.15705760812857	-3.62747629363693
H	0.63948316806955	-0.10842765879265	-4.76763465251121
H	-1.39955516355362	-1.43022779218570	-4.28762328143397
H	-1.91953025945330	-0.13158094394537	-3.18608956000011

F	1.83720411615681	0.03007540819303	4.37202469445148
F	3.31041414047691	0.26528296992847	2.50878515646737
F	2.12061552884124	2.33948373698194	3.98518501759761
F	1.94692741497959	2.00411881894781	1.67698856720698
H	-1.79485146839314	-1.79699161048940	-2.59180697474471

7j^N E = -4900.117290583997 au [PBEh-3c]
 ZPE = 0.32218991 au
 G = -4898.26591158 au

P	-0.17629887135733	0.31828530486044	0.95790058900528
C	-1.43853464225510	-0.89999902555147	1.53347111860349
C	-2.21744967542605	-0.70225029733934	2.66656829403250
C	-1.63442011164644	-2.09144549677777	0.85444088382569
C	-3.14204603402560	-1.64375638695129	3.09070234088016
C	-2.53269284265900	-3.05480254339220	1.26160393165385
C	-3.29362188988717	-2.82714060995549	2.39360897506806
C	1.42235979890689	-0.37668336602477	0.28688661588556
C	1.92376066731389	-1.58980254843666	0.72914008739329
C	2.19561137952831	0.34425751550580	-0.60487095712105
C	3.13237769157620	-2.08830006076690	0.27367979394358
C	3.41897017287614	-0.11464667221098	-1.05301481712768
C	3.88873759748542	-1.33954601945217	-0.60858624059685
C	-0.78291040192159	2.06953818386650	0.78289819385990
C	-0.92166360078311	2.96802773406951	1.84886030110219
C	-1.11387117418813	2.59469953072478	-0.46919621895963
C	-1.35030976070883	4.27449514521681	1.67009931373935
C	-1.53065914020015	3.89432396198197	-0.66929950559560
C	-1.64960492792845	4.74604354402868	0.40979983425160
F	1.25187492740491	-2.30822300492866	1.61307540272679
F	3.58083314463226	-3.25894488396439	0.69567807164927
F	5.05170451201765	-1.79613712624376	-1.04172390823937
F	4.12803145008630	0.59563196346487	-1.92378902497371
F	1.74639863204073	1.49828247990545	-1.10026060719117
F	-0.68931716145322	2.63935104157422	3.09703705063398
F	-1.47674290197150	5.07626339160689	2.71341942362858
F	-2.05438846521388	5.98921405616062	0.23467024562472
F	-1.81793238038871	4.32273115758757	-1.89418525294842
F	-1.04219263174586	1.87096838499317	-1.59912589867728
F	-2.15217654761768	0.42061811746259	3.35111429254344
F	-3.88766758578440	-1.41268367436681	4.15801026391498
F	-4.16893956670899	-3.73092494612604	2.79489843480769
F	-2.66787086882181	-4.18456803393808	0.57699211869337
F	-0.91953980357208	-2.36504132450589	-0.24990134014640
O	0.45973430185596	0.44420682272550	2.44759200728109

Si	1.84434856467056	0.87416411605530	3.33930704084277
H	-0.71912834507954	0.09321719004981	-0.38092046512455
H	0.01132318012864	-0.45837060217838	-1.98033958289469
N	0.02789326184935	-0.81537607854637	-2.94668694626291
C	0.80766220665836	-2.07920782989926	-2.94683219318862
C	0.66892441346776	0.20907419490804	-3.81217041389025
C	-1.38957716179672	-1.03855232601159	-3.32658186081396
H	0.87417752482327	-2.45164376850778	-3.96631245639229
H	1.80416616433486	-1.88128761905370	-2.56207724491268
H	0.31740428540171	-2.81357916824021	-2.31750465253105
H	1.70174685835926	0.35078762411655	-3.50989505921185
H	0.13531125711251	1.14887876505753	-3.72004308455281
H	0.63565338900362	-0.13879928737580	-4.84176027902310
H	-1.43102796907211	-1.42287589383644	-4.34281950098665
H	-1.92643875276799	-0.09673530916304	-3.26347236641949
Cl	1.30790208806606	-0.66465207117352	4.74858410655737
Cl	3.68257877607519	-0.03494660089122	2.87833447859935
Cl	1.90855598592808	2.34586494308314	4.80556473719798
Cl	2.25848392869743	2.44098768785738	1.76834685205747
H	-1.83248951416620	-1.75408858307426	-2.64100612669926