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1 CASSCF occupations and coefficients

Table 1: Active space: (14e, 13o)

State	Occupation	c^2
	HBCN$^-$	
^{1}A′	$(4a')^2(5a')^2(6a')^2(7a')^2(1a'')^2(8a')^2(9a')^2$	0.8942
	$(4a')^2(5a')^2(6a')^2(7a')^2(8a')^2(9a')^2(2a'')^2$	0.0138
X^{3}A″	$(4a')^2(5a')^2(6a')^2(7a')^2(1a'')^2(8a')^2(9a')^\alpha(2a'')^\alpha$	0.9071
	$(4a')^2(5a')^2(6a')^2(7a')^2(1a'')^2(9a')^\alpha(2a'')^\alpha(10a')^2$	0.0099
	HCCN	
^{1}A′	$(4a')^2(5a')^2(6a')^2(7a')^2(8a')^2(1a'')^2(9a')^2$	0.8632
	$(4a')^2(5a')^2(6a')^2(7a')^2(8a')^2(1a'')^2(2a'')^2$	0.0243
X^{3}A″	$(4a')^2(5a')^2(6a')^2(7a')^2(1a'')^2(8a')^2(9a')^\alpha(2a'')^\alpha$	0.8747
	$(4a')^2(5a')^2(6a')^2(7a')^2(1a'')^\alpha(8a')^2(9a')^\alpha(2a'')^\beta(3a'')^\alpha$	0.0095
	HNCN$^+$	
^{1}A′	$(4a')^2(5a')^2(6a')^2(7a')^2(8a')^2(1a'')^2(9a')^2$	0.8412
	$(4a')^2(5a')^2(6a')^2(7a')^2(8a')^2(9a')^2(2a'')^2$	0.0357
X^{3}A″	$(4a1)^2(5a1)^2(6a1)^2(7a1)^2(1b1)^2(1b2)^2(2b2)^\alpha(2b1)^\alpha$	0.8845
	$(4a1)^2(5a1)^2(6a1)^2(7a1)^2(1b2)^2(2b2)^\alpha(2b1)^\alpha(3b1)^2$	0.0091
	HAlCN$^-$	
X^{1}A′	$(7a')^2(8a')^2(9a')^2(10a')^2(11a')^2(2a'')^2(12a')^2$	0.8583
	$(7a')^2(8a')^2(9a')^2(10a')^2(11a')^2(2a'')^2(3a'')^2$	0.0517
^{3}A″	$(7a')^2(8a')^2(9a')^2(10a')^2(2a'')^2(11a')^2(12a')^\alpha(3a'')^\alpha$	0.9130
	$(7a')^2(8a')^2(9a')^2(10a')^2(2a'')^2(12a')^\alpha(3a'')^\alpha(13a')^2$	0.0123
	HSiCN	
X^{1}A′	$(7a')^2(8a')^2(9a')^2(10a')^2(11a')^2(2a'')^2(12a')^2$	0.8683
	$(7a')^2(8a')^2(9a')^2(10a')^2(11a')^2(2a'')^2(3a'')^2$	0.0359
^{3}A″	$(7a')^2(8a')^2(9a')^2(10a')^2(2a'')^2(11a')^2(12a')^\alpha(3a'')^\alpha$	0.9065
	$(7a')^2(8a')^2(9a')^2(10a')^2(2a'')^2(12a')^\alpha(3a'')^\alpha(13a')^2$	0.0132
	HPCN$^+$	
X^{1}A′	$(7a')^2(8a')^2(9a')^2(10a')^2(11a')^2(12a')^2(2a'')^2$	0.8549
	$(7a')^2(8a')^2(9a')^2(10a')^2(11a')^2(12a')^2(3a'')^2$	0.0104
^{3}A″	$(7a')^2(8a')^2(9a')^2(10a')^2(2a'')^2(11a')^2(12a')^\alpha(3a'')^\alpha$	0.8739
	$(7a')^2(8a')^2(9a')^2(10a')^2(2a'')^2(12a')^\alpha(3a'')^\alpha(13a')^2$	0.0134
	HGaCN$^-$	
X^{1}A′	$(13a')^2(14a')^2(15a')^2(16a')^2(17a')^2(5a'')^2(18a')^2$	0.8716
	$(13a')^2(14a')^2(15a')^2(16a')^2(17a')^2(5a'')^2(6a'')^2$	0.0312
^{3}A″	$(13a')^2(14a')^2(15a')^2(16a')^2(5a'')^2(17a')^2(18a')^\alpha(6a'')^\alpha$	0.9067
	$(13a')^2(14a')^2(15a')^2(16a')^2(5a'')^2(18a')^\alpha(6a'')^\alpha(19a')^2$	0.0128
	HGeCN	
X^{1}A′	$(13a')^2(14a')^2(15a')^2(16a')^2(17a')^2(5a'')^2(18a')^2$	0.8782
	$(13a')^2(14a')^2(15a')^2(16a')^2(17a')^2(5a'')^2(6a'')^2$	0.0141
^{3}A″	$(13a')^2(14a')^2(15a')^2(16a')^2(5a'')^2(17a')^2(18a')^\alpha(6a'')^\alpha$	0.9064
	$(13a')^2(14a')^2(15a')^2(16a')^2(5a'')^2(18a')^\alpha(6a'')^\alpha(19a')^2$	0.0132
	HAsCN$^+$	
X^{1}A′	$(13a')^2(14a')^2(15a')^2(16a')^2(17a')^2(5a'')^2(18a')^2$	0.8607
	$(13a')^2(14a')^2(15a')^2(16a')^2(17a')^2(18a')^2(6a'')^2$	0.0130
^{3}A″	$(13a')^2(14a')^2(15a')^2(16a')^2(5a'')^2(17a')^2(18a')^\alpha(6a'')^\alpha$	0.8750
	$(13a')^2(14a')^2(15a')^2(16a')^2(5a'')^2(18a')^\alpha(6a'')^\alpha(19a')^2$	0.0133

2 Focal point tables for XH_4 species

BH_4^- singlet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−26.9775063	−27.1216705	−27.1499106	−27.1541781	−27.1548208	−27.1549368
aug-cc-pVTZ	−26.9873528	−27.1563632	−27.1803501	−27.1862239	−27.1868491	[−27.1869651]
aug-cc-pVQZ	−26.9893815	−27.1663498	−27.1877604	−27.1940082	[−27.1946334]	[−27.1947494]
aug-cc-pV5Z	−26.9898699	−27.1696289	−27.1897198	−27.1960705	[−27.1966957]	[−27.1968117]
CBS LIMIT	[−26.9900247]	[−27.1727117]	[−27.1914181]	[−27.1978766]	[−27.1985018]	[−27.1986178]
$E_{CBS+corrections} = -27.1986178 + 0.0334594 + -0.0457323 + -0.0066525 + 0.0023451 =$ **-27.2151980**						

CH_4 singlet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−40.1996324	−40.3675495	−40.3909131	−40.3954081	−40.3958457	−40.3960056
aug-cc-pVTZ	−40.2135398	−40.4144237	−40.4343693	−40.4409302	−40.4413237	[−40.4414836]
aug-cc-pVQZ	−40.2161599	−40.4273322	−40.4447004	−40.4517214	[−40.4521149]	[−40.4522748]
aug-cc-pV5Z	−40.2168644	−40.4318157	−40.4477319	−40.4548910	[−40.4552844]	[−40.4554443]
CBS LIMIT	[−40.2171235]	[−40.4360396]	[−40.4504324]	[−40.4577363]	[−40.4581298]	[−40.4582897]
$E_{CBS+corrections} = -40.4582897 + 0.0448036 + -0.0486048 + -0.0147779 + 0.0025885 =$ **-40.4742803**						

NH_4^+ singlet at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−56.5476109	−56.7397329	−56.7576285	−56.7619876	−56.7622712	−56.7625382	−56.7625255
aug-cc-pVTZ	−56.5642278	−56.7961440	−56.8111571	−56.8180161	−56.8182284	−56.8184954	[−56.8184828]
aug-cc-pVQZ	−56.5680334	−56.8133395	−56.8258629	−56.8332750	[−56.8334874]	[−56.8337543]	[−56.8337417]
aug-cc-pV5Z	−56.5689783	−56.8193018	−56.8302173	−56.8378061	[−56.8380185]	[−56.8382854]	[−56.8382728]
CBS LIMIT	[−56.5692904]	[−56.8248782]	[−56.8341065]	[−56.8418808]	[−56.8420931]	[−56.8423601]	[−56.8423475]
$E_{CBS+corrections} = -56.8423475 + 0.0497486 + -0.0510905 + -0.0289632 + 0.0026574 =$ **-56.8699952**							

AlH_4^- singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−244.2396696	−244.3525897	−244.3857901	−244.3881447	−244.3888112	−244.3888703
aug-cc-pVTZ	−244.2504753	−244.3829536	−244.4126355	−244.4157386	−244.4164567	[−244.4165158]
aug-cc-pVQZ	−244.2537439	−244.3929073	−244.4200783	−244.4234079	[−244.4241260]	[−244.4241852]
aug-cc-pV5Z	−244.2543294	−244.3960536	−244.4218620	−244.4252610	[−244.4259791]	[−244.4260382]
CBS LIMIT	[−244.2544571]	[−244.3988681]	[−244.4232469]	[−244.4267187]	[−244.4274367]	[−244.4274959]
$E_{CBS+corrections} = -244.4274959 + 0.0239164 + -0.2793909 + -0.4368897 + 0.0053702 =$ **-245.1144898**						

SiH_4 singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−291.2503264	−291.3718194	−291.4037402	−291.4066330	−291.4073170	−291.4073905
aug-cc-pVTZ	−291.2638094	−291.4093841	−291.4387736	−291.4427881	−291.4435419	[−291.4436154]
aug-cc-pVQZ	−291.2676463	−291.4216371	−291.4487180	−291.4530562	[−291.4538100]	[−291.4538834]
aug-cc-pV5Z	−291.2683268	−291.4255827	−291.4511593	−291.4556045	[−291.4563583]	[−291.4564317]
CBS LIMIT	[−291.2684736]	[−291.4291552]	[−291.4531535]	[−291.4577108]	[−291.4584646]	[−291.4585381]
$E_{CBS+corrections} = -291.4585381 + 0.0313304 + -0.2873821 + -0.6045624 + 0.0058716 =$ **-292.3132806**						

PH_4^+ singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−342.7950569	−342.9268340	−342.9575007	−342.9610357	−342.9617282	−342.9618278
aug-cc-pVTZ	−342.8105251	−342.9721435	−343.0014352	−343.0065397	−343.0073195	[−343.0074191]
aug-cc-pVQZ	−342.8144476	−342.9863600	−343.0134917	−343.0190353	[−343.0198151]	[−343.0199147]
aug-cc-pV5Z	−342.8152510	−342.9912878	−343.0167596	−343.0224597	[−343.0232395]	[−343.0233391]
CBS LIMIT	[−342.8154579]	[−342.9958220]	[−343.0195522]	[−343.0254166]	[−343.0261964]	[−343.0262960]
$E_{CBS+corrections} = -343.0262960 + 0.0354090 + -0.2915337 + -0.8178094 + 0.0059599 =$ **-344.0942701**						

GaH_4^- singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−1925.5268528	−1925.8931339	−1925.9041000	−1925.9152156	−1925.9155879	−1925.9147134
aug-cc-pVTZ	−1925.5965818	−1926.1883995	−1926.1755030	−1926.1908990	−1926.1905503	[−1926.1896758]
aug-cc-pVQZ	−1925.5999526	−1926.2563016	−1926.2355559	−1926.2536843	[−1926.2533356]	[−1926.2524611]
aug-cc-pV5Z	−1925.6003477	−1926.2816419	−1926.2572640	−1926.2761746	[−1926.2758258]	[−1926.2749513]
CBS LIMIT	[−1925.6004002]	[−1926.3078664]	[−1926.2796777]	[−1926.2994088]	[−1926.2990601]	[−1926.2981856]
$E_{CBS+corrections} = -1926.2981856 + 0.0243128 + -0.3747981 + -18.9850990 + 0.0125759 =$ **-1945.6211940**						

GeH_4 singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2077.6486362	−2078.0160954	−2078.0287192	−2078.0380116	−2078.0382870	−2078.0378092
aug-cc-pVTZ	−2077.7189321	−2078.3146979	−2078.3063611	−2078.3198176	−2078.3196392	[−2078.3191614]
aug-cc-pVQZ	−2077.7222470	−2078.3836958	−2078.3682006	−2078.3840611	[−2078.3838827]	[−2078.3834049]
aug-cc-pV5Z	−2077.7226642	−2078.4104454	−2078.3914535	−2078.4080478	[−2078.4078694]	[−2078.4073916]
CBS LIMIT	[−2077.7227242]	[−2078.4381330]	[−2078.4154723]	[−2078.4328365]	[−2078.4326581]	[−2078.4321803]
$E_{CBS+corrections} = -2078.4321803 + 0.0299229 + -0.3927546 + -21.7716986 + 0.0124816 =$ **-2100.5542289**						

AsH_4^+ singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2236.2097670	−2236.5840537	−2236.5962143	−2236.6046942	−2236.6049527	−2236.6047049
aug-cc-pVTZ	−2236.2813766	−2236.8876383	−2236.8812420	−2236.8938719	−2236.8937950	[−2236.8935472]
aug-cc-pVQZ	−2236.2846687	−2236.9585608	−2236.9454944	−2236.9603843	[−2236.9603074]	[−2236.9600597]
aug-cc-pV5Z	−2236.2851047	−2236.9866604	−2236.9701615	−2236.9857579	[−2236.9856810]	[−2236.9854332]
CBS LIMIT	[−2236.2851713]	[−2237.0157511]	[−2236.9956508]	[−2237.0119884]	[−2237.0119115]	[−2237.0116638]
$E_{CBS+corrections} = -2237.0116638 + 0.0326841 + -0.3978563 + -24.8679369 + 0.0129656 =$ **-2262.2318072**						

3 Focal point tables for H_3XCN species

H_3BCN^- singlet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−118.7901855	−119.2040010	−119.2284185	−119.2470982	−119.2476189	−119.2493582
aug-cc-pVTZ	−118.8177417	−119.3087435	−119.3251375	−119.3504945	−119.3506321	[−119.3523715]
aug-cc-pVQZ	−118.8248039	−119.3424480	−119.3528701	−119.3797613	[−119.3798989]	[−119.3816382]
aug-cc-pV5Z	−118.8262853	−119.3541995	−119.3609842	−119.3884010	[−119.3885386]	[−119.3902780]
CBS LIMIT	[−118.8266785]	[−119.3653680]	[−119.3683364]	[−119.3963047]	[−119.3964423]	[−119.3981816]
$E_{CBS+corrections} = -119.3981816 + 0.0363041 + -0.1447676 + -0.0507375 + 0.0056365 =$ **-119.5517461**						

H_3CCN singlet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−131.9425429	−132.3823148	−132.4027294	−132.4216507	−132.4219854	−132.4238331
aug-cc-pVTZ	−131.9735801	−132.4980079	−132.5107813	−132.5369206	−132.5368326	[−132.5386804]
aug-cc-pVQZ	−131.9811768	−132.5344087	−132.5411728	−132.5689407	[−132.5688527]	[−132.5707005]
aug-cc-pV5Z	−131.9828651	−132.5472066	−132.5502367	−132.5785632	[−132.5784752]	[−132.5803230]
CBS LIMIT	[−131.9833474]	[−132.5593450]	[−132.5584575]	[−132.5873701]	[−132.5872821]	[−132.5891298]
$E_{CBS+corrections} = -132.5891298 + 0.0451276 + -0.1476904 + -0.0588622 + 0.0059244 =$ **-132.7446305**						

H_3NCN^+ singlet at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−148.2084515	−148.6788653	−148.6952728	−148.7147333	−148.7149301	−148.7170979	−148.7168026
aug-cc-pVTZ	−148.2429831	−148.8041605	−148.8127012	−148.8399927	−148.8397254	−148.8418931	[−148.8415979]
aug-cc-pVQZ	−148.2517780	−148.8444200	−148.8468948	−148.8759239	[−148.8756565]	[−148.8778243]	[−148.8775291]
aug-cc-pV5Z	−148.2536988	−148.8585207	−148.8571013	−148.8867333	[−148.8864660]	[−148.8886337]	[−148.8883385]
CBS LIMIT	[−148.2542356]	[−148.8718364]	[−148.8663312]	[−148.8965958]	[−148.8963285]	[−148.8984962]	[−148.8982010]
$E_{CBS+corrections} = -148.8982010 + 0.0479513 + -0.1500503 + -0.0730669 + 0.0060709 =$ **-149.0672960**							

H_3AlCN^- singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−336.0464312	−336.4317667	−336.4606672	−336.4775540	−336.4781248	−336.4798879
aug-cc-pVTZ	−336.0764639	−336.5328320	−336.5543096	−336.5770901	−336.5773193	[−336.5790824]
aug-cc-pVQZ	−336.0846333	−336.5664733	−336.5820470	−336.6062291	[−336.6064583]	[−336.6082214]
aug-cc-pV5Z	−336.0862290	−336.5781477	−336.5900252	−336.6147055	[−336.6149347]	[−336.6166978]
CBS LIMIT	[−336.0866163]	[−336.5891095]	[−336.5971089]	[−336.6223119]	[−336.6225411]	[−336.6243042]
$E_{CBS+corrections} = -336.6243042 + 0.0267532 + -0.3783702 + -0.4809890 + 0.0086840 =$ **-337.4482262**						

H_3SiCN singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−383.0075046	−383.4048223	−383.4320773	−383.4498138	−383.4503777	−383.4523108
aug-cc-pVTZ	−383.0405642	−383.5131393	−383.5337288	−383.5578098	−383.5580399	[−383.5599730]
aug-cc-pVQZ	−383.0493628	−383.5491144	−383.5639262	−383.5895315	[−383.5897616]	[−383.5916947]
aug-cc-pV5Z	−383.0510625	−383.5615673	−383.5725527	−383.5987006	[−383.5989307]	[−383.6008638]
CBS LIMIT	[−383.0514694]	[−383.5732563]	[−383.5802271]	[−383.6069443]	[−383.6071744]	[−383.6091075]
$E_{CBS+corrections} = -383.6091075 + 0.0327549 + -0.3863758 + -0.6486362 + 0.0091988 =$ **-384.6021658**						

H_3PCN^+ singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−434.5009449	−434.9148641	−434.9402488	−434.9596326	−434.9601704	−434.9623726
aug-cc-pVTZ	−434.5362109	−435.0306634	−435.0499309	−435.0762889	−435.0764850	[−435.0786872]
aug-cc-pVQZ	−434.5452641	−435.0685389	−435.0820683	−435.1100933	[−435.1102895]	[−435.1124916]
aug-cc-pV5Z	−434.5471093	−435.0819545	−435.0914977	−435.1201283	[−435.1203245]	[−435.1225266]
CBS LIMIT	[−434.5475816]	[−435.0945662]	[−435.0999273]	[−435.1291932]	[−435.1293894]	[−435.1315916]
$E_{CBS+corrections} = -435.1315916 + 0.0358248 + -0.3905094 + -0.8618440 + 0.0093351 =$ **-436.3387851**						

H_3GaCN^- singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2017.3307693	−2017.9766743	−2017.9822714	−2018.0087419	−2018.0088689	−2018.0097027
aug-cc-pVTZ	−2017.4188543	−2018.3394342	−2018.3173383	−2018.3529154	−2018.3519944	[−2018.3528282]
aug-cc-pVQZ	−2017.4264927	−2018.4273217	−2018.3942459	−2018.4334220	[−2018.4325010]	[−2018.4333348]
aug-cc-pV5Z	−2017.4277832	−2018.4599132	−2018.4211672	−2018.4614289	[−2018.4605080]	[−2018.4613418]
CBS LIMIT	[−2017.4280455]	[−2018.4930160]	[−2018.4483209]	[−2018.4897217]	[−2018.4888007]	[−2018.4896345]
$E_{CBS+corrections} = -2018.4896345 + 0.0270479 + -0.4740489 + -19.0289523 + 0.0158940 =$ **-2037.9496938**						

H_3GeCN singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2169.4028837	−2170.0529429	−2170.0600275	−2170.0849684	−2170.0849799	−2170.0863493
aug-cc-pVTZ	−2169.4921456	−2170.4192327	−2170.4013042	−2170.4353396	−2170.4345530	[−2170.4359224]
aug-cc-pVQZ	−2169.4997762	−2170.5081943	−2170.4799126	−2170.5172397	[−2170.5164532]	[−2170.5178226]
aug-cc-pV5Z	−2169.5010927	−2170.5421741	−2170.5083598	−2170.5467295	[−2170.5459429]	[−2170.5473123]
CBS LIMIT	[−2169.5013673]	[−2170.5767183]	[−2170.5370992]	[−2170.5765628]	[−2170.5757763]	[−2170.5771457]
$E_{CBS+corrections} = -2170.5771457 + 0.0313372 + -0.4922751 + -21.8152028 + 0.0158181 =$ **-2192.8374683**						

H_3AsCN singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2327.9155126	−2328.5779140	−2328.5842579	−2328.6093283	−2328.6092870	−2328.6111145
aug-cc-pVTZ	−2328.0064504	−2328.9489631	−2328.9321611	−2328.9664455	−2328.9657065	[−2328.9675340]
aug-cc-pVQZ	−2328.0141061	−2329.0397339	−2329.0129746	−2329.0504283	[−2329.0496893]	[−2329.0515168]
aug-cc-pV5Z	−2328.0154501	−2329.0750150	−2329.0427861	−2329.0812622	[−2329.0805232]	[−2329.0823507]
CBS LIMIT	[−2328.0157363]	[−2329.1109073]	[−2329.0729398]	[−2329.1124886]	[−2329.1117496]	[−2329.1135771]
$E_{CBS+corrections} = -2329.1135771 + 0.0332063 + -0.4971966 + -24.9111434 + 0.0163446 =$ **-2354.4723663**						

4 Focal point tables for XH_2 species

BH_2^- singlet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−25.7147405	−25.8193299	−25.8452454	−25.8492182	−25.8501090	−25.8503142
aug-cc-pVTZ	−25.7208108	−25.8438979	−25.8662613	−25.8715187	−25.8723848	[−25.8725900]
aug-cc-pVQZ	−25.7223670	−25.8515545	−25.8716630	−25.8772328	[−25.8780988]	[−25.8783040]
aug-cc-pV5Z	−25.7227349	−25.8541951	−25.8731255	−25.8787957	[−25.8796617]	[−25.8798669]
CBS LIMIT	[−25.7228488]	[−25.8566935]	[−25.8743878]	[−25.8801634]	[−25.8810294]	[−25.8812346]

$E_{CBS+corrections} = -25.8812346 + 0.0126331 + -0.0447000 + -0.0066929 + 0.0019784 =$ **-25.9180160**

BH_2^- singlet at the CCSD(T)/aug-cc-pVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−25.7147252	−25.8192961	−25.8451922	−25.8491609	−25.8500510	−25.8502564
aug-cc-pVTZ	−25.7208320	−25.8439168	−25.8662618	−25.8715155	−25.8723812	[−25.8725866]
aug-cc-pVQZ	−25.7223919	−25.8515798	−25.8716699	−25.8772360	[−25.8781018]	[−25.8783072]
aug-cc-pV5Z	−25.7227613	−25.8542237	−25.8731354	−25.8788021	[−25.8796678]	[−25.8798732]
CBS LIMIT	[−25.7228760]	[−25.8567247]	[−25.8744000]	[−25.8801722]	[−25.8810379]	[−25.8812433]

$E_{CBS+corrections} = -25.8812433 + 0.0126734 + -0.0498599 + -0.0066929 + 0.0019825 =$ **-25.9231403**

BH_2^- triplet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−25.7364551	−25.8261913	−25.8475658	−25.8504092	−25.8511218	−25.8512251
aug-cc-pVTZ	−25.7429090	−25.8490933	−25.8681767	−25.8722318	−25.8729641	[−25.8730674]
aug-cc-pVQZ	−25.7445732	−25.8559095	−25.8734084	−25.8777448	[−25.8784771]	[−25.8785804]
aug-cc-pV5Z	−25.7450974	−25.8579913	−25.8748298	−25.8792388	[−25.8799711]	[−25.8800744]
CBS LIMIT	[−25.7453384]	[−25.8598665]	[−25.8760122]	[−25.8804974]	[−25.8812297]	[−25.8813330]

$E_{CBS+corrections} = -25.8813330 + 0.0135507 + -0.0450241 + -0.0067095 + 0.0019770 =$ **-25.9175390**

BH_2^- triplet at the CCSD(T)/aug-cc-pVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−25.7364425	−25.8261533	−25.8475201	−25.8503589	−25.8510704	−25.8511736
aug-cc-pVTZ	−25.7429274	−25.8490987	−25.8681789	−25.8722293	−25.8729608	[−25.8730640]
aug-cc-pVQZ	−25.7445951	−25.8559180	−25.8734160	−25.8777473	[−25.8784789]	[−25.8785821]
aug-cc-pV5Z	−25.7451223	−25.8579961	−25.8748396	−25.8792432	[−25.8799747]	[−25.8800779]
CBS LIMIT	[−25.7453659]	[−25.8598670]	[−25.8760238]	[−25.8805032]	[−25.8812347]	[−25.8813379]

$E_{CBS+corrections} = -25.8813379 + 0.0135880 + -0.0502140 + -0.0066680 + 0.0018646 =$ **-25.9227672**

CH_2 singlet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−38.8843411	−38.9998730	−39.0277549	−39.0312792	−39.0320646	−39.0322454
aug-cc-pVTZ	−38.8932487	−39.0343692	−39.0594900	−39.0645916	−39.0654139	[−39.0655947]
aug-cc-pVQZ	−38.8953136	−39.0446802	−39.0675368	−39.0730005	[−39.0738228]	[−39.0740036]
aug-cc-pV5Z	−38.8958241	−39.0483100	−39.0698825	−39.0754669	[−39.0762892]	[−39.0764700]
CBS LIMIT	[−38.8959918]	[−39.0517504]	[−39.0719755]	[−39.0776866]	[−39.0785089]	[−39.0786897]

$E_{CBS+corrections} = -39.0786897 + 0.0166099 + -0.0473660 + -0.0149366 + 0.0023634 =$ **-39.1220190**

CH_2 singlet at the CCSD(T)/aug-cc-pVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−38.8843662	−38.9998311	−39.0276884	−39.0312074	−39.0319931	−39.0321736
aug-cc-pVTZ	−38.8933168	−39.0343908	−39.0594926	−39.0645878	−39.0654111	[−39.0655916]
aug-cc-pVQZ	−38.8953845	−39.0447093	−39.0675473	−39.0730043	[−39.0738276]	[−39.0740082]
aug-cc-pV5Z	−38.8958958	−39.0483413	−39.0698953	−39.0754730	[−39.0762963]	[−39.0764769]
CBS LIMIT	[−38.8960637]	[−39.0517836]	[−39.0719903]	[−39.0776947]	[−39.0785179]	[−39.0786985]
$E_{CBS+corrections} = -39.0786985 + 0.0166665 + -0.0527970 + -0.0149365 + 0.0023663 =$ **-39.1273993**						

CH_2 triplet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−38.9229243	−39.0247119	−39.0456957	−39.0480025	−39.0484786	−39.0485581
aug-cc-pVTZ	−38.9325345	−39.0574688	−39.0763534	−39.0800454	−39.0805638	[−39.0806433]
aug-cc-pVQZ	−38.9346801	−39.0668997	−39.0839850	−39.0880086	[−39.0885270]	[−39.0886065]
aug-cc-pV5Z	−38.9352137	−39.0701107	−39.0861671	−39.0902949	[−39.0908133]	[−39.0908928]
CBS LIMIT	[−38.9353903]	[−39.0730965]	[−39.0880733]	[−39.0923104]	[−39.0928288]	[−39.0929083]
$E_{CBS+corrections} = -39.0929083 + 0.0172781 + -0.0479730 + -0.0148365 + 0.0021589 =$ **-39.1362808**						

CH_2 triplet at the CCSD(T)/aug-cc-pVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−38.9229190	−39.0246694	−39.0456339	−39.0479360	−39.0484109	−39.0484901
aug-cc-pVTZ	−38.9325681	−39.0574861	−39.0763558	−39.0800422	−39.0805596	[−39.0806388]
aug-cc-pVQZ	−38.9347158	−39.0669234	−39.0839937	−39.0880117	[−39.0885291]	[−39.0886083]
aug-cc-pV5Z	−38.9352499	−39.0701367	−39.0861780	−39.0903001	[−39.0908175]	[−39.0908967]
CBS LIMIT	[−38.9354267]	[−39.0731245]	[−39.0880861]	[−39.0923175]	[−39.0928349]	[−39.0929141]
$E_{CBS+corrections} = -39.0929141 + 0.0173228 + -0.0534583 + -0.0148369 + 0.0021608 =$ **-39.1417258**						

NH_2^+ singlet at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−55.1423733	−55.2678710	−55.2963014	−55.2996824	−55.3004875	−55.3007115	−55.3007543
aug-cc-pVTZ	−55.1549453	−55.3119829	−55.3383568	−55.3434629	−55.3443711	−55.3445951	[−55.3446378]
aug-cc-pVQZ	−55.1581675	−55.3257758	−55.3499809	−55.3554970	[−55.3564052]	[−55.3566292]	[−55.3566720]
aug-cc-pV5Z	−55.1589329	−55.3307018	−55.3535080	−55.3591721	[−55.3600804]	[−55.3603044]	[−55.3603471]
CBS LIMIT	[−55.1591713]	[−55.3353055]	[−55.3566440]	[−55.3624635]	[−55.3633717]	[−55.3635957]	[−55.3636385]
$E_{CBS+corrections} = -55.3636385 + 0.0178934 + -0.0497581 + -0.0293105 + 0.0026114 =$ **-55.4222023**							

NH_2^+ singlet at the CCSD(T)/aug-cc-pVQZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−55.1424480	−55.2678409	−55.2962541	−55.2996314	−55.3004384	−55.3006619	−55.3007045
aug-cc-pVTZ	−55.1550490	−55.3119941	−55.3383580	−55.3434580	−55.3443690	−55.3445924	[−55.3446351]
aug-cc-pVQZ	−55.1582754	−55.3257958	−55.3499920	−55.3555018	[−55.3564127]	[−55.3566362]	[−55.3566788]
aug-cc-pV5Z	−55.1590415	−55.3307237	−55.3535213	−55.3591790	[−55.3600899]	[−55.3603134]	[−55.3603561]
CBS LIMIT	[−55.1592801]	[−55.3353286]	[−55.3566590]	[−55.3624719]	[−55.3633828]	[−55.3636063]	[−55.3636489]
$E_{CBS+corrections} = -55.3636489 + 0.0179446 + -0.0555153 + -0.0293103 + 0.0026148 =$ **-55.4279152**							

NH_2^+ triplet at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−55.2128606	−55.3262824	−55.3472700	−55.3492908	−55.3496718	−55.3497513	−55.3498042
aug-cc-pVTZ	−55.2255360	−55.3681105	−55.3871103	−55.3905646	−55.3909941	−55.3910736	[−55.3911265]
aug-cc-pVQZ	−55.2288191	−55.3807845	−55.3979192	−55.4017359	[−55.4021654]	[−55.4022449]	[−55.4022978]
aug-cc-pV5Z	−55.2296126	−55.3851385	−55.4011129	−55.4050519	[−55.4054814]	[−55.4055608]	[−55.4056138]
CBS LIMIT	[−55.2298656]	[−55.3891270]	[−55.4038840]	[−55.4079513]	[−55.4083808]	[−55.4084602]	[−55.4085132]
$E_{CBS+corrections} = -55.4085132 + 0.0170982 + -0.0504387 + -0.0291538 + 0.0023657 =$ **-55.4686417**							

NH_2^+ triplet at the CCSD(T)/aug-cc-pVQZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−55.2129176	−55.3262685	−55.3472347	−55.3492508	−55.3496308	−55.3497099	−55.3497627
aug-cc-pVTZ	−55.2256182	−55.3681290	−55.3871137	−55.3905615	−55.3909901	−55.3910692	[−55.3911220]
aug-cc-pVQZ	−55.2289039	−55.3808084	−55.3979292	−55.4017391	[−55.4021677]	[−55.4022468]	[−55.4022996]
aug-cc-pV5Z	−55.2296980	−55.3851632	−55.4011243	−55.4050563	[−55.4054849]	[−55.4055640]	[−55.4056169]
CBS LIMIT	[−55.2299512]	[−55.3891521]	[−55.4038965]	[−55.4079566]	[−55.4083852]	[−55.4084643]	[−55.4085172]
$E_{CBS+corrections} = -55.4085172 + 0.0171382 + -0.0562517 + -0.0291542 + 0.0023677 =$ **-55.4744171**							

AlH_2^- singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−243.0299455	−243.1148306	−243.1427448	−243.1454619	−243.1462458	−243.1463699
aug-cc-pVTZ	−243.0379229	−243.1372287	−243.1621608	−243.1657244	−243.1665372	[−243.1666613]
aug-cc-pVQZ	−243.0401394	−243.1444651	−243.1671604	−243.1709661	[−243.1717789]	[−243.1719030]
aug-cc-pV5Z	−243.0405863	−243.1470186	−243.1684877	−243.1723696	[−243.1731824]	[−243.1733065]
CBS LIMIT	[−243.0406991]	[−243.1493417]	[−243.1695244]	[−243.1734862]	[−243.1742990]	[−243.1744231]
$E_{CBS+corrections} = -243.1744231 + 0.0085994 + -0.2794625 + -0.4372596 + 0.0048732 =$ **-243.8776726**						

AlH_2^- singlet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−243.0299550	−243.1148321	−243.1427246	−243.1454383	−243.1462206	−243.1463446
aug-cc-pVTZ	−243.0379372	−243.1372470	−243.1621579	−243.1657183	−243.1665298	[−243.1666537]
aug-cc-pVQZ	−243.0401624	−243.1444944	−243.1671697	−243.1709722	[−243.1717836]	[−243.1719075]
aug-cc-pV5Z	−243.0406101	−243.1470487	−243.1684983	−243.1723769	[−243.1731883]	[−243.1733123]
CBS LIMIT	[−243.0407229]	[−243.1493717]	[−243.1695353]	[−243.1734938]	[−243.1743052]	[−243.1744291]
$E_{CBS+corrections} = -243.1744291 + 0.0087066 + -0.3497936 + -0.4372588 + 0.0048767 =$ **-243.9478981**						

AlH_2^- triplet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−243.0306796	−243.1004398	−243.1228599	−243.1250283	−243.1257907	−243.1258426
aug-cc-pVTZ	−243.0387703	−243.1205708	−243.1413066	−243.1442331	−243.1450585	[−243.1451104]
aug-cc-pVQZ	−243.0411824	−243.1271101	−243.1463321	−243.1494810	[−243.1503064]	[−243.1503582]
aug-cc-pV5Z	−243.0416445	−243.1292127	−243.1475785	−243.1507970	[−243.1516224]	[−243.1516742]
CBS LIMIT	[−243.0417541]	[−243.1310433]	[−243.1485110]	[−243.1518024]	[−243.1526277]	[−243.1526796]
$E_{CBS+corrections} = -243.1526796 + 0.0095191 + -0.2787946 + -0.4372180 + 0.0048358 =$ **-243.8543373**						

AlH_2^- triplet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−243.0306947	−243.1004444	−243.1228517	−243.1250165	−243.1257773	−243.1258290
aug-cc-pVTZ	−243.0387892	−243.1205851	−243.1413080	−243.1442309	−243.1450547	[−243.1451064]
aug-cc-pVQZ	−243.0412046	−243.1271281	−243.1463382	−243.1494834	[−243.1503072]	[−243.1503589]
aug-cc-pV5Z	−243.0416674	−243.1292313	−243.1475856	−243.1508002	[−243.1516240]	[−243.1516757]
CBS LIMIT	[−243.0417770]	[−243.1310622]	[−243.1485184]	[−243.1518059]	[−243.1526297]	[−243.1526814]
$E_{CBS+corrections} = -243.1526814 + 0.0096195 + -0.3491222 + -0.4372187 + 0.0048403 =$ **-243.9245625**						

SiH_2 singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−290.0227265	−290.1156962	−290.1451510	−290.1479172	−290.1486447	−290.1487614
aug-cc-pVTZ	−290.0321103	−290.1434014	−290.1704785	−290.1743967	−290.1751997	[−290.1753164]
aug-cc-pVQZ	−290.0347481	−290.1525544	−290.1773871	−290.1816220	[−290.1824251]	[−290.1825417]
aug-cc-pV5Z	−290.0352811	−290.1558018	−290.1792528	−290.1835921	[−290.1843952]	[−290.1845118]
CBS LIMIT	[−290.0354162]	[−290.1587847]	[−290.1807860]	[−290.1852348]	[−290.1860379]	[−290.1861545]
$E_{CBS+corrections} = -290.1861545 + 0.0116859 + -0.2874584 + -0.6053129 + 0.0054334 =$ **-291.0618065**						

SiH_2 singlet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−290.0227339	−290.1156864	−290.1451263	−290.1478881	−290.1486143	−290.1487308
aug-cc-pVTZ	−290.0321356	−290.1434182	−290.1704799	−290.1743934	−290.1751954	[−290.1753119]
aug-cc-pVQZ	−290.0347782	−290.1525768	−290.1773952	−290.1816253	[−290.1824273]	[−290.1825438]
aug-cc-pV5Z	−290.0353121	−290.1558252	−290.1792622	−290.1835966	[−290.1843986]	[−290.1845150]
CBS LIMIT	[−290.0354472]	[−290.1588085]	[−290.1807960]	[−290.1852399]	[−290.1860419]	[−290.1861583]
$E_{CBS+corrections} = -290.1861583 + 0.0117708 + -0.3582956 + -0.6053126 + 0.0054361 =$ **-291.1325595**						

SiH_2 triplet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−290.0139019	−290.0914000	−290.1146727	−290.1169846	−290.1177151	−290.1177639
aug-cc-pVTZ	−290.0234162	−290.1166502	−290.1387112	−290.1420862	−290.1429182	[−290.1429670]
aug-cc-pVQZ	−290.0263429	−290.1249910	−290.1455260	−290.1492095	[−290.1500415]	[−290.1500903]
aug-cc-pV5Z	−290.0268378	−290.1277118	−290.1472387	−290.1510236	[−290.1518556]	[−290.1519044]
CBS LIMIT	[−290.0269385]	[−290.1301480]	[−290.1486170]	[−290.1525084]	[−290.1533404]	[−290.1533892]
$E_{CBS+corrections} = -290.1533892 + 0.0121069 + -0.2867679 + -0.6048071 + 0.0053511 =$ **-291.0275062**						

SiH_2 triplet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−290.0139188	−290.0913988	−290.1146551	−290.1169628	−290.1176915	−290.1177402
aug-cc-pVTZ	−290.0234471	−290.1166688	−290.1387135	−290.1420838	−290.1429142	[−290.1429628]
aug-cc-pVQZ	−290.0263773	−290.1250134	−290.1455333	−290.1492119	[−290.1500423]	[−290.1500909]
aug-cc-pV5Z	−290.0268728	−290.1277349	−290.1472469	−290.1510269	[−290.1518573]	[−290.1519059]
CBS LIMIT	[−290.0269736]	[−290.1301712]	[−290.1486258]	[−290.1525122]	[−290.1533425]	[−290.1533912]
$E_{CBS+corrections} = -290.1533912 + 0.0122006 + -0.3576352 + -0.6048078 + 0.0053533 =$ **-291.0982802**						

PH_2^+ singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−341.5354942	−341.6354428	−341.6658323	−341.6686831	−341.6693757	−341.6695053
aug-cc-pVTZ	−341.5466627	−341.6695528	−341.6985619	−341.7028735	−341.7036850	[−341.7038145]
aug-cc-pVQZ	−341.5496860	−341.6804522	−341.7072603	−341.7119475	[−341.7127590]	[−341.7128885]
aug-cc-pV5Z	−341.5503265	−341.6844660	−341.7097587	−341.7145818	[−341.7153933]	[−341.7155228]
CBS LIMIT	[−341.5504988]	[−341.6881773]	[−341.7118801]	[−341.7168457]	[−341.7176573]	[−341.7177868]
$E_{CBS+corrections} = -341.7177868 + 0.0135592 + -0.2912795 + -0.8189407 + 0.0056255 =$ **-342.8088223**						

PH_2^+ singlet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−341.5355086	−341.6354333	−341.6658136	−341.6686613	−341.6693533	−341.6694826
aug-cc-pVTZ	−341.5466923	−341.6695638	−341.6985647	−341.7028724	−341.7036834	[−341.7038128]
aug-cc-pVQZ	−341.5497174	−341.6804649	−341.7072653	−341.7119485	[−341.7127595]	[−341.7128889]
aug-cc-pV5Z	−341.5503586	−341.6844792	−341.7097645	−341.7145835	[−341.7153945]	[−341.7155238]
CBS LIMIT	[−341.5505310]	[−341.6881906]	[−341.7118863]	[−341.7168477]	[−341.7176588]	[−341.7177881]
$E_{CBS+corrections} = -341.7177881 + 0.0135993 + -0.3657516 + -0.8189405 + 0.0056275 =$ **-342.8832534**						

PH_2^+ triplet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−341.5310075	−341.6161740	−341.6400352	−341.6425398	−341.6432704	−341.6433256
aug-cc-pVTZ	−341.5423728	−341.6475128	−341.6708354	−341.6746990	−341.6755622	[−341.6756174]
aug-cc-pVQZ	−341.5455292	−341.6573739	−341.6791089	−341.6833581	[−341.6842213]	[−341.6842765]
aug-cc-pV5Z	−341.5460993	−341.6607986	−341.6813779	−341.6857602	[−341.6866234]	[−341.6866786]
CBS LIMIT	[−341.5462250]	[−341.6639191]	[−341.6832861]	[−341.6878079]	[−341.6886712]	[−341.6887264]
$E_{CBS+corrections} = -341.6887264 + 0.0132835 + -0.2908575 + -0.8182699 + 0.0055147 =$ **-342.7790557**						

PH_2^+ triplet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−341.5310309	−341.6161682	−341.6400171	−341.6425182	−341.6432475	−341.6433025
aug-cc-pVTZ	−341.5424113	−341.6475267	−341.6708383	−341.6746975	−341.6755596	[−341.6756145]
aug-cc-pVQZ	−341.5455698	−341.6573899	−341.6791149	−341.6833596	[−341.6842216]	[−341.6842766]
aug-cc-pV5Z	−341.5461405	−341.6608148	−341.6813847	−341.6857623	[−341.6866243]	[−341.6866793]
CBS LIMIT	[−341.5462663]	[−341.6639352]	[−341.6832932]	[−341.6878103]	[−341.6886723]	[−341.6887273]
$E_{CBS+corrections} = -341.6887273 + 0.0133412 + -0.3653864 + -0.8182702 + 0.0055165 =$ **-342.8535263**						

GaH_2^- singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−1924.3345896	−1924.6689228	−1924.6733481	−1924.6845772	−1924.6849151	−1924.6841362
aug-cc-pVTZ	−1924.4033094	−1924.9576142	−1924.9387548	−1924.9543085	−1924.9538950	[−1924.9531162]
aug-cc-pVQZ	−1924.4059790	−1925.0233004	−1924.9968809	−1925.0151834	[−1925.0147700]	[−1925.0139911]
aug-cc-pV5Z	−1924.4062556	−1925.0480483	−1925.0181657	−1925.0372493	[−1925.0368359]	[−1925.0360570]
CBS LIMIT	[−1924.4062876]	[−1925.0737550]	[−1925.0402390]	[−1925.0601422]	[−1925.0597288]	[−1925.0589499]
$E_{CBS+corrections} = -1925.0589499 + 0.0082295 + -0.3738500 + -18.9876385 + 0.0120926 =$ **-1944.4001162**						

GaH_2^- singlet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−1924.3345738	−1924.6689399	−1924.6733402	−1924.6845684	−1924.6849056	−1924.6841263
aug-cc-pVTZ	−1924.4032905	−1924.9576383	−1924.9387537	−1924.9543068	−1924.9538927	[−1924.9531133]
aug-cc-pVQZ	−1924.4059617	−1925.0233276	−1924.9968831	−1925.0151851	[−1925.0147709]	[−1925.0139915]
aug-cc-pV5Z	−1924.4062385	−1925.0480756	−1925.0181682	−1925.0372512	[−1925.0368370]	[−1925.0360577]
CBS LIMIT	[−1924.4062705]	[−1925.0737823]	[−1925.0402416]	[−1925.0601442]	[−1925.0597300]	[−1925.0589507]
$E_{CBS+corrections} = -1925.0589507 + 0.0083191 + -0.6551541 + -18.9876410 + 0.0120940 =$ **-1944.6813327**						

GaH_2^- triplet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−1924.3292156	−1924.6477102	−1924.6496291	−1924.6598888	−1924.6603068	−1924.6593187
aug-cc-pVTZ	−1924.3975636	−1924.9337535	−1924.9139758	−1924.9282719	−1924.9280071	[−1924.9270190]
aug-cc-pVQZ	−1924.4007325	−1924.9988313	−1924.9722095	−1924.9891507	[−1924.9888858]	[−1924.9878978]
aug-cc-pV5Z	−1924.4010226	−1925.0231842	−1924.9934047	−1925.0111030	[−1925.0108381]	[−1925.0098501]
CBS LIMIT	[−1924.4010518]	[−1925.0484596]	[−1925.0153672]	[−1925.0338599]	[−1925.0335950]	[−1925.0326070]
$E_{CBS+corrections} = -1925.0326070 + 0.0096830 + -0.3737047 + -18.9859104 + 0.0120428 =$ **-1944.3704962**						

GaH_2^- triplet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−1924.3292098	−1924.6477196	−1924.6496283	−1924.6598868	−1924.6603043	−1924.6593158
aug-cc-pVTZ	−1924.3975565	−1924.9337655	−1924.9139764	−1924.9282716	−1924.9280061	[−1924.9270177]
aug-cc-pVQZ	−1924.4007261	−1924.9988437	−1924.9722108	−1924.9891510	[−1924.9888855]	[−1924.9878971]
aug-cc-pV5Z	−1924.4010162	−1925.0231965	−1924.9934060	−1925.0111033	[−1925.0108379]	[−1925.0098495]
CBS LIMIT	[−1924.4010455]	[−1925.0484718]	[−1925.0153684]	[−1925.0338602]	[−1925.0335947]	[−1925.0326063]
$E_{CBS+corrections} = -1925.0326063 + 0.0097050 + -0.6549387 + -18.9859157 + 0.0120501 =$ **-1944.6517056**						

GeH_2 singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2076.4483989	−2076.7853047	−2076.7926045	−2076.8016562	−2076.8018915	−2076.8014696
aug-cc-pVTZ	−2076.5168211	−2077.0762804	−2077.0625045	−2077.0758261	−2077.0755748	[−2077.0751530]
aug-cc-pVQZ	−2076.5196542	−2077.1430200	−2077.1222057	−2077.1379329	[−2077.1376816]	[−2077.1372598]
aug-cc-pV5Z	−2076.5199420	−2077.1691605	−2077.1449796	−2077.1614438	[−2077.1611925]	[−2077.1607706]
CBS LIMIT	[−2076.5199745]	[−2077.1963172]	[−2077.1686041]	[−2077.1858415]	[−2077.1855902]	[−2077.1851683]
$E_{CBS+corrections} = -2077.1851683 + 0.0109809 + -0.3925174 + -21.7755557 + 0.0120580 =$ **-2099.3302026**						

GeH_2 singlet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2076.4483948	−2076.7853121	−2076.7926000	−2076.8016497	−2076.8018847	−2076.8014626
aug-cc-pVTZ	−2076.5168185	−2077.0762945	−2077.0625059	−2077.0758255	−2077.0755739	[−2077.0751518]
aug-cc-pVQZ	−2076.5196516	−2077.1430351	−2077.1222082	−2077.1379335	[−2077.1376818]	[−2077.1372598]
aug-cc-pV5Z	−2076.5199394	−2077.1691757	−2077.1449822	−2077.1614445	[−2077.1611928]	[−2077.1607708]
CBS LIMIT	[−2076.5199720]	[−2077.1963324]	[−2077.1686069]	[−2077.1858423]	[−2077.1855906]	[−2077.1851686]
$E_{CBS+corrections} = -2077.1851686 + 0.0110143 + -0.6743888 + -21.7755588 + 0.0120594 =$ **-2099.6120424**						

GeH_2 triplet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2076.4312335	−2076.7525968	−2076.7569759	−2076.7651643	−2076.7654933	−2076.7649390
aug-cc-pVTZ	−2076.4998762	−2077.0411293	−2077.0259946	−2077.0381635	−2077.0380489	[−2077.0374946]
aug-cc-pVQZ	−2076.5027476	−2077.1070217	−2077.0854998	−2077.1000034	[−2077.0998889]	[−2077.0993346]
aug-cc-pV5Z	−2076.5030398	−2077.1327668	−2077.1081679	−2077.1233883	[−2077.1232738]	[−2077.1227195]
CBS LIMIT	[−2076.5030729]	[−2077.1595045]	[−2077.1316774]	[−2077.1476498]	[−2077.1475353]	[−2077.1469810]
$E_{CBS+corrections} = -2077.1469810 + 0.0115431 + -0.3921333 + -21.7728769 + 0.0119737 =$ **-2099.2884744**						

GeH_2 triplet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2076.4312342	−2076.7526043	−2076.7569742	−2076.7651607	−2076.7654892	−2076.7649347
aug-cc-pVTZ	−2076.4998779	−2077.0411408	−2077.0259962	−2077.0381632	−2077.0380481	[−2077.0374936]
aug-cc-pVQZ	−2076.5027492	−2077.1070337	−2077.0855020	−2077.1000037	[−2077.0998886]	[−2077.0993341]
aug-cc-pV5Z	−2076.5030416	−2077.1327788	−2077.1081702	−2077.1233886	[−2077.1232735]	[−2077.1227190]
CBS LIMIT	[−2076.5030747]	[−2077.1595164]	[−2077.1316796]	[−2077.1476501]	[−2077.1475350]	[−2077.1469804]
$E_{CBS+corrections} = -2077.1469804 + 0.0115673 + -0.6739740 + -21.7728809 + 0.0119748 =$ **-2099.5702932**						

AsH_2^+ singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2234.9879821	−2235.3292559	−2235.3379052	−2235.3457373	−2235.3459520	−2235.3457454
aug-cc-pVTZ	−2235.0577076	−2235.6241621	−2235.6138277	−2235.6258180	−2235.6256881	[−2235.6254815]
aug-cc-pVQZ	−2235.0605500	−2235.6924483	−2235.6754898	−2235.6897061	[−2235.6895763]	[−2235.6893696]
aug-cc-pV5Z	−2235.0608566	−2235.7197808	−2235.6995312	−2235.7144442	[−2235.7143143]	[−2235.7141077]
CBS LIMIT	[−2235.0608937]	[−2235.7481728]	[−2235.7244704]	[−2235.7401142]	[−2235.7399844]	[−2235.7397777]
$E_{CBS+corrections} = -2235.7397777 + 0.0124726 + -0.3972538 + -24.8727738 + 0.0126306 =$ **-2260.9847022**						

AsH_2^+ singlet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2234.9879894	−2235.3292610	−2235.3379024	−2235.3457324	−2235.3459469	−2235.3457401
aug-cc-pVTZ	−2235.0577171	−2235.6241723	−2235.6138299	−2235.6258177	−2235.6256876	[−2235.6254808]
aug-cc-pVQZ	−2235.0605596	−2235.6924591	−2235.6754927	−2235.6897064	[−2235.6895764]	[−2235.6893696]
aug-cc-pV5Z	−2235.0608663	−2235.7197915	−2235.6995341	−2235.7144445	[−2235.7143145]	[−2235.7141076]
CBS LIMIT	[−2235.0609034]	[−2235.7481833]	[−2235.7244732]	[−2235.7401144]	[−2235.7399844]	[−2235.7397776]
$E_{CBS+corrections} = -2235.7397776 + 0.0124878 + -0.6841431 + -24.8727761 + 0.0126319 =$ **-2261.2715771**						

AsH_2^+ triplet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2234.9730469	−2235.3000913	−2235.3052349	−2235.3123394	−2235.3126616	−2235.3123506
aug-cc-pVTZ	−2235.0430998	−2235.5923332	−2235.5797733	−2235.5907770	−2235.5907697	[−2235.5904587]
aug-cc-pVQZ	−2235.0459569	−2235.6597662	−2235.6411614	−2235.6543337	[−2235.6543264]	[−2235.6540155]
aug-cc-pV5Z	−2235.0462635	−2235.6866890	−2235.6650703	−2235.6789220	[−2235.6789146]	[−2235.6786037]
CBS LIMIT	[−2235.0463004]	[−2235.7146510]	[−2235.6898703]	[−2235.7044346]	[−2235.7044272]	[−2235.7041163]
$E_{CBS+corrections} = -2235.7041163 + 0.0122175 + -0.3967199 + -24.8698392 + 0.0125275 =$ **-2260.9459305**						

AsH_2^+ triplet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2234.9730565	−2235.3000968	−2235.3052332	−2235.3123352	−2235.3126568	−2235.3123457
aug-cc-pVTZ	−2235.0431113	−2235.5923430	−2235.5797759	−2235.5907767	−2235.5907688	[−2235.5904577]
aug-cc-pVQZ	−2235.0459685	−2235.6597764	−2235.6411646	−2235.6543340	[−2235.6543261]	[−2235.6540150]
aug-cc-pV5Z	−2235.0462753	−2235.6866990	−2235.6650736	−2235.6789221	[−2235.6789143]	[−2235.6786032]
CBS LIMIT	[−2235.0463122]	[−2235.7146607]	[−2235.6898734]	[−2235.7044346]	[−2235.7044268]	[−2235.7041156]
$E_{CBS+corrections} = -2235.7041156 + 0.0122412 + -0.6837016 + -24.8698414 + 0.0125285 =$ **-2261.2328890**						

5 Focal point tables for HXCN species

$HBCN^-$ singlet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−117.5208005	−117.8996208	−117.9201653	−117.9398612	−117.9406916	−117.9428783
aug-cc-pVTZ	−117.5444776	−117.9942360	−118.0074454	−118.0336567	−118.0340848	[−118.0362715]
aug-cc-pVQZ	−117.5510366	−118.0256807	−118.0332714	−118.0609837	[−118.0614118]	[−118.0635985]
aug-cc-pV5Z	−117.5523643	−118.0368015	−118.0409118	−118.0691561	[−118.0695842]	[−118.0717708]
CBS LIMIT	[−117.5527012]	[−118.0474133]	[−118.0478720]	[−118.0766744]	[−118.0771025]	[−118.0792891]
$E_{CBS+corrections} = -118.0792891 + 0.0154590 + -0.1437480 + -0.0507786 + 0.0052065 =$ **-118.2531502**						

$HBCN^-$ singlet at the CCSD(T)/aug-cc-pVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−117.5211202	−117.8992823	−117.9199365	−117.9395277	−117.9403649	−117.9425308
aug-cc-pVTZ	−117.5449806	−117.9941819	−118.0075294	−118.0336264	−118.0340651	[−118.0362310]
aug-cc-pVQZ	−117.5515608	−118.0256803	−118.0334172	−118.0610140	[−118.0614528]	[−118.0636187]
aug-cc-pV5Z	−117.5528924	−118.0368148	−118.0410736	−118.0692017	[−118.0696405]	[−118.0718064]
CBS LIMIT	[−117.5532302]	[−118.0474376]	[−118.0480474]	[−118.0767328]	[−118.0771716]	[−118.0793375]
$E_{CBS+corrections} = -118.0793375 + 0.0155257 + -0.1603270 + -0.0507811 + 0.0052082 =$ **-118.2697117**						

$HBCN^-$ triplet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−117.5420483	−117.9115572	−117.9276818	−117.9458968	−117.9465169	−117.9484100
aug-cc-pVTZ	−117.5659761	−118.0052794	−118.0150635	−118.0397910	−118.0400428	[−118.0419359]
aug-cc-pVQZ	−117.5725816	−118.0361855	−118.0408302	−118.0670588	[−118.0673106]	[−118.0692037]
aug-cc-pV5Z	−117.5739220	−118.0470317	−118.0484223	−118.0751770	[−118.0754288]	[−118.0773219]
CBS LIMIT	[−117.5742633]	[−118.0573463]	[−118.0553226]	[−118.0826293]	[−118.0828812]	[−118.0847742]
$E_{CBS+corrections} = -118.0847742 + 0.0159921 + -0.1442906 + -0.0507196 + 0.0051169 =$ **-118.2586754**						

$HBCN^-$ triplet at the CCSD(T)/aug-cc-pVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−117.5423689	−117.9112186	−117.9274694	−117.9455794	−117.9462020	−117.9480744
aug-cc-pVTZ	−117.5664701	−118.0052129	−118.0151506	−118.0397623	−118.0400201	[−118.0418925]
aug-cc-pVQZ	−117.5730945	−118.0361704	−118.0409758	−118.0670874	[−118.0673452]	[−118.0692176]
aug-cc-pV5Z	−117.5744384	−118.0470300	−118.0485833	−118.0752203	[−118.0754781]	[−118.0773504]
CBS LIMIT	[−117.5747805]	[−118.0573556]	[−118.0554970]	[−118.0826851]	[−118.0829430]	[−118.0848153]
$E_{CBS+corrections} = -118.0848153 + 0.0160571 + -0.1609118 + -0.0507228 + 0.0051183 =$ **-118.2752745**						

HCCN singlet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−130.6356190	−131.0300166	−131.0528215	−131.0739988	−131.0750477	−131.0776123
aug-cc-pVTZ	−130.6622959	−131.1342424	−131.1499547	−131.1781206	−131.1787886	[−131.1813532]
aug-cc-pVQZ	−130.6694585	−131.1682928	−131.1783262	−131.2080874	[−131.2087554]	[−131.2113200]
aug-cc-pV5Z	−130.6709846	−131.1803089	−131.1867788	−131.2171047	[−131.2177728]	[−131.2203373]
CBS LIMIT	[−130.6713978]	[−131.1917280]	[−131.1944592]	[−131.2253775]	[−131.2260456]	[−131.2286101]
$E_{CBS+corrections} = -131.2286101 + 0.0178643 + -0.1465320 + -0.0590372 + 0.0056765 =$ **-131.4106385**						

HCCN singlet at the CCSD(T)/aug-cc-pVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−130.6360220	−131.0296910	−131.0525782	−131.0736362	−131.0746947	−131.0772329
aug-cc-pVTZ	−130.6628967	−131.1342285	−131.1500552	−131.1780898	−131.1787718	[−131.1813100]
aug-cc-pVQZ	−130.6700771	−131.1683331	−131.1784896	−131.2081181	[−131.2088002]	[−131.2113384]
aug-cc-pV5Z	−130.6716071	−131.1803641	−131.1869598	−131.2171523	[−131.2178343]	[−131.2203725]
CBS LIMIT	[−130.6720215]	[−131.1917958]	[−131.1946556]	[−131.2254397]	[−131.2261217]	[−131.2286599]
$E_{CBS+corrections} = -131.2286599 + 0.0179129 + -0.1633875 + -0.0590394 + 0.0056785 =$ **-131.4274954**						

HCCN triplet at the CCSD(T)/aug-cc-pVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−130.6581234	−131.0543767	−131.0736066	−131.0929624	−131.0937444	−131.0960078
aug-cc-pVTZ	−130.6857430	−131.1580492	−131.1706399	−131.1970211	−131.1974005	[−131.1996639]
aug-cc-pVQZ	−130.6929704	−131.1914952	−131.1987176	−131.2267303	[−131.2271097]	[−131.2293731]
aug-cc-pV5Z	−130.6945154	−131.2031656	−131.2070124	−131.2355939	[−131.2359733]	[−131.2382367]
CBS LIMIT	[−130.6949355]	[−131.2142090]	[−131.2145141]	[−131.2436924]	[−131.2440719]	[−131.2463352]
$E_{CBS+corrections} = -131.2463352 + 0.0175004 + -0.1472253 + -0.0589235 + 0.0055296 =$ **-131.4294540**						

HCCN triplet at the CCSD(T)/aug-cc-pVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−130.6582685	−131.0540249	−131.0733261	−131.0925843	−131.0933649	−131.0956039
aug-cc-pVTZ	−130.6860857	−131.1580283	−131.1707170	−131.1969912	−131.1973718	[−131.1996109]
aug-cc-pVQZ	−130.6933275	−131.1915294	−131.1988554	−131.2267601	[−131.2271407]	[−131.2293798]
aug-cc-pV5Z	−130.6948758	−131.2032163	−131.2071676	−131.2356405	[−131.2360211]	[−131.2382602]
CBS LIMIT	[−130.6952968]	[−131.2142745]	[−131.2146852]	[−131.2437542]	[−131.2441349]	[−131.2463739]
$E_{CBS+corrections} = -131.2463739 + 0.0175130 + -0.1641347 + -0.0589269 + 0.0055319 =$ **-131.4463906**						

$HNCN^+$ singlet at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−146.8840756	−147.3007059	−147.3291826	−147.3545955	−147.3560437	−147.3595945	−147.3590918
aug-cc-pVTZ	−146.9150949	−147.4142159	−147.4352540	−147.4681596	−147.4692199	−147.4727707	[−147.4722680]
aug-cc-pVQZ	−146.9234678	−147.4513754	−147.4667051	−147.5013112	[−147.5023715]	[−147.5059223]	[−147.5054196]
aug-cc-pV5Z	−146.9252445	−147.4644975	−147.4761506	−147.5113738	[−147.5124341]	[−147.5159849]	[−147.5154822]
CBS LIMIT	[−146.9257230]	[−147.4768795]	[−147.4846750]	[−147.5205458]	[−147.5216060]	[−147.5251568]	[−147.5246542]
$E_{CBS+corrections} = -147.5246542 + 0.0184187 + -0.1487880 + -0.0733884 + 0.0060798 =$ **-147.7223321**							

$HNCN^+$ singlet at the CCSD(T)/aug-cc-pVQZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−146.8846751	−147.3005394	−147.3290150	−147.3542448	−147.3557047	−147.3592167	−147.3587260
aug-cc-pVTZ	−146.9158717	−147.4143422	−147.4354173	−147.4681253	−147.4692021	−147.4727141	[−147.4722234]
aug-cc-pVQZ	−146.9242646	−147.4515613	−147.4669387	−147.5013455	[−147.5024223]	[−147.5059343]	[−147.5054436]
aug-cc-pV5Z	−146.9260454	−147.4647001	−147.4764041	−147.5114269	[−147.5125037]	[−147.5160157]	[−147.5155251]
CBS LIMIT	[−146.9265250]	[−147.4770964]	[−147.4849461]	[−147.5206155]	[−147.5216923]	[−147.5252042]	[−147.5247136]
$E_{CBS+corrections} = -147.5247136 + 0.0184517 + -0.1659465 + -0.0733894 + 0.0060835 =$ **-147.7395143**							

$HNCN^+$ triplet at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−146.9530941	−147.3476411	−147.3750391	−147.3931327	−147.3942753	−147.3960838	−147.3959802
aug-cc-pVTZ	−146.9855576	−147.4605638	−147.4810473	−147.5062438	−147.5070780	−147.5088865	[−147.5087829]
aug-cc-pVQZ	−146.9939813	−147.4969912	−147.5121059	−147.5389412	[−147.5397754]	[−147.5415839]	[−147.5414803]
aug-cc-pV5Z	−146.9957866	−147.5096815	−147.5213415	−147.5487581	[−147.5495922]	[−147.5514008]	[−147.5512972]
CBS LIMIT	[−146.9962790]	[−147.5215943]	[−147.5296297]	[−147.5576561]	[−147.5584903]	[−147.5602988]	[−147.5601952]
$E_{CBS+corrections} = -147.5601952 + 0.0186638 + -0.1494077 + -0.0732593 + 0.0057584 =$ **-147.7584400**							

$HNCN^+$ triplet at the CCSD(T)/aug-cc-pVQZ geometry							
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)	CCSDTQ
aug-cc-pVDZ	−146.9532426	−147.3472747	−147.3747714	−147.3927725	−147.3939129	−147.3957073	−147.3956059
aug-cc-pVTZ	−146.9858900	−147.4604975	−147.4811143	−147.5062084	−147.5070434	−147.5088378	[−147.5087363]
aug-cc-pVQZ	−146.9943334	−147.4969866	−147.5122445	−147.5389768	[−147.5398119]	[−147.5416063]	[−147.5415048]
aug-cc-pV5Z	−146.9961427	−147.5096927	−147.5214985	−147.5488115	[−147.5496465]	[−147.5514410]	[−147.5513395]
CBS LIMIT	[−146.9966361]	[−147.5216188]	[−147.5298028]	[−147.5577250]	[−147.5585600]	[−147.5603545]	[−147.5602530]
$E_{CBS+corrections} = -147.5602530 + 0.0187726 + -0.1666084 + -0.0732628 + 0.0057603 =$ **-147.7755912**							

$HAlCN^-$ singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−334.8362532	−335.1960537	−335.2190807	−335.2368469	−335.2374477	−335.2393858
aug-cc-pVTZ	−334.8632091	−335.2887790	−335.3047257	−335.3284815	−335.3286888	[−335.3306269]
aug-cc-pVQZ	−334.8702932	−335.3195790	−335.3299265	−335.3551033	[−335.3553105]	[−335.3572487]
aug-cc-pV5Z	−334.8717452	−335.3306750	−335.3374599	−335.3631463	[−335.3633535]	[−335.3652917]
CBS LIMIT	[−334.8721196]	[−335.3411675]	[−335.3442148]	[−335.3704358]	[−335.3706430]	[−335.3725812]
$E_{CBS+corrections} = -335.3725812 + 0.0117726 + -0.3785587 + -0.4814206 + 0.0081565 =$ **-336.2126314**						

$HAlCN^-$ singlet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−334.8365755	−335.1956910	−335.2188716	−335.2365357	−335.2371421	−335.2390590
aug-cc-pVTZ	−334.8637109	−335.2886787	−335.3048052	−335.3284494	−335.3286660	[−335.3305828]
aug-cc-pVQZ	−334.8708185	−335.3195346	−335.3300714	−335.3551355	[−335.3553521]	[−335.3572689]
aug-cc-pV5Z	−334.8722748	−335.3306450	−335.3376218	−335.3631949	[−335.3634116]	[−335.3653284]
CBS LIMIT	[−334.8726501]	[−335.3411491]	[−335.3443909]	[−335.3704981]	[−335.3707147]	[−335.3726315]
$E_{CBS+corrections} = -335.3726315 + 0.0118680 + -0.4601880 + -0.4814210 + 0.0081583 =$ **-336.2942143**						

HAlCN$^-$ triplet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−334.8273719	−335.1720401	−335.1893690	−335.2064834	−335.2071112	−335.2089522
aug-cc-pVTZ	−334.8547876	−335.2630465	−335.2746807	−335.2977564	−335.2980506	[−335.2998916]
aug-cc-pVQZ	−334.8621195	−335.2933339	−335.3000779	−335.3245688	[−335.3248629]	[−335.3267040]
aug-cc-pV5Z	−334.8635890	−335.3040001	−335.3075566	−335.3325548	[−335.3328490]	[−335.3346901]
CBS LIMIT	[−334.8639574]	[−335.3140175]	[−335.3142297]	[−335.3397603]	[−335.3400544]	[−335.3418955]
$E_{CBS+corrections} = -335.3418955 + 0.0124671 + -0.3777020 + -0.4810671 + 0.0081269 =$ **-336.1800706**						

HAlCN$^-$ triplet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−334.8277178	−335.1717031	−335.1891907	−335.2062010	−335.2068332	−335.2086530
aug-cc-pVTZ	−334.8552969	−335.2629491	−335.2747667	−335.2977280	−335.2980240	[−335.2998439]
aug-cc-pVQZ	−334.8626480	−335.2932857	−335.3002221	−335.3245972	[−335.3248933]	[−335.3267131]
aug-cc-pV5Z	−334.8641215	−335.3039659	−335.3077170	−335.3325989	[−335.3328949]	[−335.3347148]
CBS LIMIT	[−334.8644909]	[−335.3139947]	[−335.3144040]	[−335.3398175]	[−335.3401136]	[−335.3419334]
$E_{CBS+corrections} = -335.3419334 + 0.0124339 + -0.4593633 + -0.4810706 + 0.0081286 =$ **-336.2618048**						

HSiCN singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−381.7844609	−382.1557371	−382.1793688	−382.1978909	−382.1984669	−382.2006094
aug-cc-pVTZ	−381.8134021	−382.2540352	−382.2709606	−382.2958925	−382.2960939	[−382.2982364]
aug-cc-pVQZ	−381.8210261	−382.2868521	−382.2980992	−382.3245666	[−382.3247680]	[−382.3269105]
aug-cc-pV5Z	−381.8225788	−382.2986274	−382.3061762	−382.3331917	[−382.3333931]	[−382.3355357]
CBS LIMIT	[−381.8229758]	[−382.3097499]	[−382.3134184]	[−382.3410091]	[−382.3412105]	[−382.3433530]
$E_{CBS+corrections} = -382.3433530 + 0.0139050 + -0.3865043 + -0.6494673 + 0.0087319 =$ **-383.3566877**						

HSiCN singlet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−381.7848309	−382.1553573	−382.1791521	−382.1975633	−382.1981462	−382.2002633
aug-cc-pVTZ	−381.8139557	−382.2539310	−382.2710484	−382.2958587	−382.2960712	[−382.2981883]
aug-cc-pVQZ	−381.8216047	−382.2868066	−382.2982557	−382.3246004	[−382.3248129]	[−382.3269300]
aug-cc-pV5Z	−381.8231616	−382.2985974	−382.3063507	−382.3332430	[−382.3334555]	[−382.3355726]
CBS LIMIT	[−381.8235595]	[−382.3097326]	[−382.3136083]	[−382.3410752]	[−382.3412877]	[−382.3434048]
$E_{CBS+corrections} = -382.3434048 + 0.0139816 + -0.4686752 + -0.6494684 + 0.0087337 =$ **-383.4388330**						

HSiCN triplet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−381.7660127	−382.1222695	−382.1403810	−382.1582146	−382.1588842	−382.1609229
aug-cc-pVTZ	−381.7952388	−382.2183646	−382.2309823	−382.2551938	−382.2555338	[−382.2575725]
aug-cc-pVQZ	−381.8032082	−382.2505300	−382.2581881	−382.2839317	[−382.2842717]	[−382.2863104]
aug-cc-pV5Z	−381.8047368	−382.2618140	−382.2661440	−382.2924373	[−382.2927773]	[−382.2948160]
CBS LIMIT	[−381.8050996]	[−382.2724119]	[−382.2732501]	[−382.3001203]	[−382.3004603]	[−382.3024990]
$E_{CBS+corrections} = -382.3024990 + 0.0141923 + -0.3857527 + -0.6488476 + 0.0086769 =$ **-383.3142301**						

HSiCN triplet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−381.7664014	−382.1219067	−382.1401779	−382.1578985	−382.1585725	−382.1605858
aug-cc-pVTZ	−381.7958026	−382.2182669	−382.2310738	−382.2551608	−382.2555092	[−382.2575225]
aug-cc-pVQZ	−381.8037959	−382.2504891	−382.2583469	−382.2839647	[−382.2843131]	[−382.2863265]
aug-cc-pV5Z	−381.8053286	−382.2617884	−382.2663206	−382.2924876	[−382.2928360]	[−382.2948494]
CBS LIMIT	[−381.8056923]	[−382.2723990]	[−382.2734421]	[−382.3001852]	[−382.3005336]	[−382.3025470]
$E_{CBS+corrections} = -382.3025470 + 0.0142846 + -0.4679592 + -0.6488513 + 0.0086785 =$ **-383.3963944**						

$HPCN^+$ singlet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−433.2562468	−433.6426788	−433.6666798	−433.6886251	−433.6893209	−433.6920859
aug-cc-pVTZ	−433.2869973	−433.7468698	−433.7644600	−433.7934079	−433.7937286	[−433.7964937]
aug-cc-pVQZ	−433.2951158	−433.7813726	−433.7932134	−433.8238182	[−433.8241390]	[−433.8269040]
aug-cc-pV5Z	−433.2967793	−433.7938417	−433.8018480	−433.8330547	[−433.8333754]	[−433.8361405]
CBS LIMIT	[−433.2972079]	[−433.8056074]	[−433.8095907]	[−433.8414288]	[−433.8417496]	[−433.8445146]
$E_{CBS+corrections} = -433.8445146 + 0.0148775 + -0.3902583 + -0.8630454 + 0.0089869 =$ **-435.0739539**						

$HPCN^+$ singlet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−433.2567451	−433.6423610	−433.6665005	−433.6882897	−433.6889935	−433.6917206
aug-cc-pVTZ	−433.2876774	−433.7468344	−433.7645955	−433.7933745	−433.7937077	[−433.7964348]
aug-cc-pVQZ	−433.2958198	−433.7813950	−433.7934169	−433.8238516	[−433.8241848]	[−433.8269119]
aug-cc-pV5Z	−433.2974873	−433.7938797	−433.8020698	−433.8331058	[−433.8334390]	[−433.8361661]
CBS LIMIT	[−433.2979168]	[−433.8056583]	[−433.8098283]	[−433.8414950]	[−433.8418283]	[−433.8445553]
$E_{CBS+corrections} = -433.8445553 + 0.0149187 + -0.4760701 + -0.8630470 + 0.0089881 =$ **-435.1597657**						

$HPCN^+$ triplet at the CCSD(T)/aug-cc-pV(T+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−433.2318621	−433.6084965	−433.6275787	−433.6484751	−433.6494046	−433.6520339
aug-cc-pVTZ	−433.2629405	−433.7102247	−433.7237675	−433.7517304	−433.7523265	[−433.7549558]
aug-cc-pVQZ	−433.2712511	−433.7438890	−433.7522329	−433.7818887	[−433.7824848]	[−433.7851141]
aug-cc-pV5Z	−433.2728659	−433.7558426	−433.7606779	−433.7909490	[−433.7915451]	[−433.7941744]
CBS LIMIT	[−433.2732554]	[−433.7670792]	[−433.7682333]	[−433.7991501]	[−433.7997462]	[−433.8023754]
$E_{CBS+corrections} = -433.8023754 + 0.0143110 + -0.3898372 + -0.8623382 + 0.0088931 =$ **-435.0313466**						

$HPCN^+$ triplet at the CCSD(T)/aug-cc-pV(Q+d)Z geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−433.2323986	−433.6081233	−433.6273890	−433.6481385	−433.6490726	−433.6516640
aug-cc-pVTZ	−433.2636591	−433.7101327	−433.7238954	−433.7516961	−433.7523011	[−433.7548925]
aug-cc-pVQZ	−433.2719940	−433.7438553	−433.7524311	−433.7819230	[−433.7825280]	[−433.7851194]
aug-cc-pV5Z	−433.2736130	−433.7558247	−433.7608951	−433.7910015	[−433.7916065]	[−433.7941979]
CBS LIMIT	[−433.2740033]	[−433.7670744]	[−433.7684669]	[−433.7992181]	[−433.7998231]	[−433.8024145]
$E_{CBS+corrections} = -433.8024145 + 0.0143783 + -0.4756813 + -0.8623403 + 0.0088945 =$ **-435.1171633**						

$HGaCN^-$ singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2016.1409268	−2016.7576677	−2016.7558986	−2016.7829279	−2016.7829916	−2016.7839926
aug-cc-pVTZ	−2016.2276588	−2017.1133920	−2017.0843161	−2017.1205198	−2017.1194772	[−2017.1204783]
aug-cc-pVQZ	−2016.2345837	−2017.1989675	−2017.1592020	−2017.1990230	[−2017.1979804]	[−2017.1989815]
aug-cc-pV5Z	−2016.2357512	−2017.2309718	−2017.1857012	−2017.2266116	[−2017.2255691]	[−2017.2265701]
CBS LIMIT	[−2016.2359880]	[−2017.2635619]	[−2017.2125154]	[−2017.2545689]	[−2017.2535264]	[−2017.2545274]
$E_{CBS+corrections} = -2017.2545274 + 0.0112709 + -0.4731484 + -19.0320948 + 0.0153830 =$ **-2036.7331167**						

$HGaCN^-$ singlet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2016.1410818	−2016.7574777	−2016.7557781	−2016.7827455	−2016.7828123	−2016.7838001
aug-cc-pVTZ	−2016.2279071	−2017.1133603	−2017.0843671	−2017.1205043	−2017.1194667	[−2017.1204544]
aug-cc-pVQZ	−2016.2348384	−2017.1989613	−2017.1592839	−2017.1990384	[−2017.1980008]	[−2017.1989885]
aug-cc-pV5Z	−2016.2360076	−2017.2309737	−2017.1857927	−2017.2266366	[−2017.2255990]	[−2017.2265867]
CBS LIMIT	[−2016.2362449]	[−2017.2635710]	[−2017.2126156]	[−2017.2546025]	[−2017.2535649]	[−2017.2545526]
$E_{CBS+corrections} = -2017.2545526 + 0.0113367 + -0.7655280 + -19.0320904 + 0.0153836 =$ **-2037.0254507**						

$HGaCN^-$ triplet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2016.1215854	−2016.7230117	−2016.7187675	−2016.7447911	−2016.7449533	−2016.7457419
aug-cc-pVTZ	−2016.2086012	−2017.0768993	−2017.0469854	−2017.0819411	−2017.0810827	[−2017.0818713]
aug-cc-pVQZ	−2016.2156827	−2017.1618929	−2017.1219524	−2017.1604557	[−2017.1595972]	[−2017.1603859]
aug-cc-pV5Z	−2016.2168701	−2017.1935828	−2017.1484251	−2017.1880024	[−2017.1871439]	[−2017.1879326]
CBS LIMIT	[−2016.2171093]	[−2017.2258247]	[−2017.1751931]	[−2017.2158972]	[−2017.2150388]	[−2017.2158275]
$E_{CBS+corrections} = -2017.2158275 + 0.0123883 + -0.4729853 + -19.0293906 + 0.0153448 =$ **-2036.6904703**						

$HGaCN^-$ triplet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2016.1217436	−2016.7228448	−2016.7186750	−2016.7446350	−2016.7447997	−2016.7455748
aug-cc-pVTZ	−2016.2088423	−2017.0768717	−2017.0470409	−2017.0819292	−2017.0810745	[−2017.0818495]
aug-cc-pVQZ	−2016.2159277	−2017.1618853	−2017.1220320	−2017.1604677	[−2017.1596130]	[−2017.1603880]
aug-cc-pV5Z	−2016.2171165	−2017.1935818	−2017.1485126	−2017.1880221	[−2017.1871674]	[−2017.1879424]
CBS LIMIT	[−2016.2173563]	[−2017.2258295]	[−2017.1752878]	[−2017.2159241]	[−2017.2150694]	[−2017.2158444]
$E_{CBS+corrections} = -2017.2158444 + 0.01241978 + -0.7652880 + -19.0294046 + 0.0153454 =$ **-2036.9827718**						

HGeCN singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2168.2093725	−2168.8318005	−2168.8322206	−2168.8576889	−2168.8576399	−2168.8592061
aug-cc-pVTZ	−2168.2965417	−2169.1901221	−2169.1652626	−2169.1999552	−2169.1990433	[−2169.2006095]
aug-cc-pVQZ	−2168.3037013	−2169.2767518	−2169.2416852	−2169.2796808	[−2169.2787688]	[−2169.2803351]
aug-cc-pV5Z	−2168.3048942	−2169.3101217	−2169.2696617	−2169.3087093	[−2169.3077973]	[−2169.3093636]
CBS LIMIT	[−2168.3051327]	[−2169.3441196]	[−2169.2980010]	[−2169.3381523]	[−2169.3372403]	[−2169.3388066]
$E_{CBS+corrections} = -2169.3388066 + 0.0131424 + -0.4920014 + -21.8196383 + 0.0153678 =$ **-2191.6219361**						

HGeCN singlet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2168.2095981	−2168.8315974	−2168.8321154	−2168.8575119	−2168.8574678	−2168.8590175
aug-cc-pVTZ	−2168.2968631	−2169.1900752	−2169.1653273	−2169.1999419	−2169.1990369	[−2169.2005865]
aug-cc-pVQZ	−2168.3040266	−2169.2767268	−2169.2417770	−2169.2796941	[−2169.2787890]	[−2169.2803387]
aug-cc-pV5Z	−2168.3052211	−2169.3101038	−2169.2697622	−2169.3087311	[−2169.3078260]	[−2169.3093757]
CBS LIMIT	[−2168.3054601]	[−2169.3441081]	[−2169.2981095]	[−2169.3381819]	[−2169.3372768]	[−2169.3388265]

$E_{CBS+corrections} = -2169.3388265 + 0.0131713 + -0.7848688 + -21.8196417 + 0.0153684 =$ **-2191.9147974**

HGeCN triplet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2168.1794477	−2168.7863951	−2168.7849427	−2168.8094492	−2168.8095608	−2168.8109665
aug-cc-pVTZ	−2168.2670799	−2169.1425873	−2169.1174210	−2169.1509182	−2169.1502323	[−2169.1516379]
aug-cc-pVQZ	−2168.2743056	−2169.2284991	−2169.1937601	−2169.2304989	[−2169.2298130]	[−2169.2312186]
aug-cc-pV5Z	−2168.2755076	−2169.2615123	−2169.2216594	−2169.2594339	[−2169.2587480]	[−2169.2601536]
CBS LIMIT	[−2168.2757474]	[−2169.2951279]	[−2169.2499096]	[−2169.2887707]	[−2169.2880847]	[−2169.2894904]

$E_{CBS+corrections} = -2169.2894904 + 0.0135094 + -0.4915971 + -21.8163019 + 0.0153109 =$ **-2191.5685690**

HGeCN triplet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2168.1796771	−2168.7862075	−2168.7848465	−2168.8092788	−2168.8093937	−2168.8107827
aug-cc-pVTZ	−2168.2674009	−2169.1425512	−2169.1174887	−2169.1509055	−2169.1502247	[−2169.1516137]
aug-cc-pVQZ	−2168.2746302	−2169.2284839	−2169.1938537	−2169.2305116	[−2169.2298308]	[−2169.2312198]
aug-cc-pV5Z	−2168.2758336	−2169.2615039	−2169.2217613	−2169.2594546	[−2169.2587738]	[−2169.2601628]
CBS LIMIT	[−2168.2760740]	[−2169.2951255]	[−2169.2500191]	[−2169.2887988]	[−2169.2881180]	[−2169.2895069]

$E_{CBS+corrections} = -2169.2895069 + 0.0134374 + -0.7844096 + -21.8163134 + 0.0153114 =$ **-2191.8614811**

$HAsCN^+$ singlet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2326.7063699	−2327.3413671	−2327.3421011	−2327.3691061	−2327.3690927	−2327.3714473
aug-cc-pVTZ	−2326.7950682	−2327.7033038	−2327.6802806	−2327.7166172	−2327.7158577	[−2327.7182123]
aug-cc-pVQZ	−2326.8022496	−2327.7913531	−2327.7584412	−2327.7979485	[−2327.7971890]	[−2327.7995436]
aug-cc-pV5Z	−2326.8034611	−2327.8258415	−2327.7876120	−2327.8281462	[−2327.8273867]	[−2327.8297413]
CBS LIMIT	[−2326.8037070]	[−2327.8610008]	[−2327.8171921]	[−2327.8588038]	[−2327.8580443]	[−2327.8603989]

$E_{CBS+corrections} = -2327.8603989 + 0.0138675 + -0.4964965 + -24.9165866 + 0.0159920 =$ **-2353.2436225**

$HAsCN^+$ singlet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2326.7066833	−2327.3411797	−2327.3420172	−2327.3689239	−2327.3689165	−2327.3712463
aug-cc-pVTZ	−2326.7954771	−2327.7032755	−2327.6803726	−2327.7166032	−2327.7158520	[−2327.7181819]
aug-cc-pVQZ	−2326.8026632	−2327.7913478	−2327.7585619	−2327.7979625	[−2327.7972113]	[−2327.7995411]
aug-cc-pV5Z	−2326.8038761	−2327.8258431	−2327.7877414	−2327.8281685	[−2327.8274174]	[−2327.8297472]
CBS LIMIT	[−2326.8041224]	[−2327.8610086]	[−2327.8173296]	[−2327.8588339]	[−2327.8580827]	[−2327.8604125]

$E_{CBS+corrections} = -2327.8604125 + 0.0138717 + -0.7944278 + -24.9165916 + 0.0159925 =$ **-2353.5415678**

$HAsCN^+$ triplet at the CCSD(T)/aug-cc-pwCVTZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2326.6724946	−2327.2954533	−2327.2950452	−2327.3209376	−2327.3212409	−2327.3234066
aug-cc-pVTZ	−2326.7616756	−2327.6550159	−2327.6320990	−2327.6672226	−2327.6668383	[−2327.6690040]
aug-cc-pVQZ	−2326.7689005	−2327.7423350	−2327.7100428	−2327.7483051	[−2327.7479207]	[−2327.7500864]
aug-cc-pV5Z	−2326.7701167	−2327.7764576	−2327.7390949	−2327.7783759	[−2327.7779916]	[−2327.7801573]
CBS LIMIT	[−2326.7703629]	[−2327.8112284]	[−2327.7685459]	[−2327.8088957]	[−2327.8085114]	[−2327.8106771]
$E_{CBS+corrections} = -2327.8106771 + 0.0133123 + -0.4959836 + -24.9134249 + 0.0159116 =$ **-2353.1908616**						

$HAsCN^+$ triplet at the CCSD(T)/aug-cc-pwCVQZ geometry						
	SCF	MP2	CCSD	CCSD(T)	CCSDT	CCSDT(Q)
aug-cc-pVDZ	−2326.6728363	−2327.2952597	−2327.2949600	−2327.3207517	−2327.3210569	−2327.3231974
aug-cc-pVTZ	−2326.7621139	−2327.6549844	−2327.6321942	−2327.6672081	−2327.6668278	[−2327.6689683]
aug-cc-pVQZ	−2326.7693434	−2327.7423269	−2327.7101681	−2327.7483197	[−2327.7479394]	[−2327.7500799]
aug-cc-pV5Z	−2326.7705611	−2327.7764564	−2327.7392292	−2327.7783991	[−2327.7780188]	[−2327.7801593]
CBS LIMIT	[−2326.7708077]	[−2327.8112335]	[−2327.7686885]	[−2327.8089269]	[−2327.8085466]	[−2327.8106871]
$E_{CBS+corrections} = -2327.8106871 + 0.0133297 + -0.7939822 + -24.9134276 + 0.0159121 =$ **-2353.4888553**						

6 Focal point tables of ΔE_{st} for the HXCN species

ΔE_{st} for $HBCN^-$ at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+13.33	−5.84	−2.77	−0.93	−0.13	−0.18	[+3.47]
aug-cc-pVTZ	+13.49	−6.56	−2.15	−0.93	−0.11	[−0.18]	[+3.55]
aug-cc-pVQZ	+13.52	−6.93	−1.85	−0.93	[−0.11]	[−0.18]	[+3.52]
aug-cc-pV5Z	+13.53	−7.11	−1.71	−0.93	[−0.11]	[−0.18]	[+3.48]
CBS LIMIT	[+13.53]	[−7.30]	[−1.56]	[−0.94]	[−0.11]	[−0.18]	[+3.44]
$\Delta E_{ST} = 3.44 + -0.33 + 0.34 + -0.04 + 0.06 =$ **3.47**							

ΔE_{st} for HCCN at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+14.12	+1.16	−2.24	−1.14	−0.17	−0.19	[+11.54]
aug-cc-pVTZ	+14.71	+0.23	−1.96	−1.12	−0.18	[−0.19]	[+11.49]
aug-cc-pVQZ	+14.75	−0.19	−1.76	−1.10	[−0.18]	[−0.19]	[+11.33]
aug-cc-pV5Z	+14.77	−0.42	−1.65	−1.09	[−0.18]	[−0.19]	[+11.23]
CBS LIMIT	[+14.77]	[−0.66]	[−1.52]	[−1.09]	[−0.18]	[−0.19]	[+11.12]
$\Delta E_{ST} = 11.12 + 0.23 + 0.44 + -0.07 + 0.09 =$ **11.81**							

ΔE_{st} for $HNCN^+$ at the CCSD(T)/aug-cc-pVTZ geometry								
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	+δ CCSDTQ	NET
aug-cc-pVDZ	+43.31	−13.86	−0.68	−4.59	−0.19	−1.09	+0.25	[+23.15]
aug-cc-pVTZ	+44.22	−15.13	−0.35	−4.84	−0.14	[−1.09]	[+0.25]	[+22.91]
aug-cc-pVQZ	+44.25	−15.62	−0.13	−4.88	[−0.14]	[−1.09]	[+0.25]	[+22.63]
aug-cc-pV5Z	+44.27	−15.91	+0.00	−4.90	[−0.14]	[−1.09]	[+0.25]	[+22.47]
CBS LIMIT	[+44.27]	[−16.22]	[+0.15]	[−4.92]	[−0.14]	[−1.09]	[+0.25]	[+22.30]
$\Delta E_{ST} = 22.30 + -0.15 + 0.39 + -0.08 + 0.20 =$ **22.66**								

ΔE_{st} for $HAlCN^-$ at the CCSD(T)/aug-cc-pV(T+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−5.57	−9.50	−3.58	−0.41	+0.02	−0.06	[−19.10]
aug-cc-pVTZ	−5.28	−10.86	−2.71	−0.43	+0.05	[−0.06]	[−19.29]
aug-cc-pVQZ	−5.13	−11.34	−2.26	−0.43	[+0.05]	[−0.06]	[−19.17]
aug-cc-pV5Z	−5.12	−11.62	−2.03	−0.43	[+0.05]	[−0.06]	[−19.20]
CBS LIMIT	[−5.12]	[−11.92]	[−1.78]	[−0.43]	[+0.05]	[−0.06]	[−19.26]
$\Delta E_{ST} = -19.26 + -0.44 + -0.54 + -0.22 + 0.02 =$ **-20.43**							

ΔE_{st} for HSiCN at the CCSD(T)/aug-cc-pV(T+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−11.58	−9.42	−3.46	−0.43	+0.06	−0.07	[−24.90]
aug-cc-pVTZ	−11.40	−10.99	−2.70	−0.45	+0.09	[−0.07]	[−25.52]
aug-cc-pVQZ	−11.18	−11.61	−2.25	−0.45	[+0.09]	[−0.07]	[−25.48]
aug-cc-pV5Z	−11.20	−11.90	−2.02	−0.45	[+0.09]	[−0.07]	[−25.55]
CBS LIMIT	[−11.22]	[−12.21]	[−1.78]	[−0.45]	[+0.09]	[−0.07]	[−25.64]
$\Delta E_{ST} = -25.64 + -0.18 + -0.47 + -0.39 + 0.03 =$ **-26.64**							

ΔE_{st} for $HPCN^+$ at the CCSD(T)/aug-cc-pV(T+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−15.30	−6.15	−3.09	−0.66	+0.15	−0.09	[−25.13]
aug-cc-pVTZ	−15.10	−7.90	−2.54	−0.62	+0.17	[−0.09]	[−26.07]
aug-cc-pVQZ	−14.98	−8.55	−2.19	−0.60	[+0.17]	[−0.09]	[−26.22]
aug-cc-pV5Z	−15.01	−8.84	−1.99	−0.59	[+0.17]	[−0.09]	[−26.33]
CBS LIMIT	[−15.03]	[−9.15]	[−1.78]	[−0.58]	[+0.17]	[−0.09]	[−26.44]
$\Delta E_{ST} = -26.44 + 0.36 + -0.26 + -0.44 + 0.06 =$ **-26.74**							

ΔE_{st} for $HGaCN^-$ at the CCSD(T)/aug-cc-pwCVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−12.14	−9.61	−1.55	−0.63	+0.06	−0.13	[−24.00]
aug-cc-pVTZ	−11.96	−10.94	−0.53	−0.78	+0.12	[−0.13]	[−24.23]
aug-cc-pVQZ	−11.86	−11.40	−0.11	−0.83	[+0.12]	[−0.13]	[−24.22]
aug-cc-pV5Z	−11.85	−11.61	+0.07	−0.84	[+0.12]	[−0.13]	[−24.25]
CBS LIMIT	[−11.85]	[−11.83]	[+0.26]	[−0.85]	[+0.12]	[−0.13]	[−24.28]
$\Delta E_{ST} = -24.28 + -0.70 + -0.10 + -1.70 + 0.02 =$ **-26.76**							

ΔE_{st} for HGeCN at the CCSD(T)/aug-cc-pwCVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−18.78	−9.71	−1.18	−0.60	+0.10	−0.10	[−30.27]
aug-cc-pVTZ	−18.49	−11.34	−0.19	−0.75	+0.14	[−0.10]	[−30.73]
aug-cc-pVQZ	−18.45	−11.83	+0.21	−0.79	[+0.14]	[−0.10]	[−30.82]
aug-cc-pV5Z	−18.44	−12.06	+0.38	−0.80	[+0.14]	[−0.10]	[−30.88]
CBS LIMIT	[−18.44]	[−12.30]	[+0.56]	[−0.81]	[+0.14]	[−0.10]	[−30.95]
$\Delta E_{ST} = -30.95 + -0.23 + -0.25 + -2.09 + 0.04 =$ **-33.49**							

ΔE_{st} for $HAsCN^+$ at the CCSD(T)/aug-cc-pwCVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	−21.26	−7.55	−0.72	−0.70	+0.20	−0.12	[−30.15]
aug-cc-pVTZ	−20.95	−9.35	+0.07	−0.76	+0.24	[−0.12]	[−30.88]
aug-cc-pVQZ	−20.93	−9.83	+0.39	−0.78	[+0.24]	[−0.12]	[−31.03]
aug-cc-pV5Z	−20.92	−10.06	+0.54	−0.79	[+0.24]	[−0.12]	[−31.11]
CBS LIMIT	[−20.92]	[−10.31]	[+0.71]	[−0.79]	[+0.24]	[−0.12]	[−31.20]
$\Delta E_{ST} = -31.20 + 0.35 + -0.32 + -1.98 + 0.05 =$ **-33.11**							

7 Focal point tables of ΔE_{st} for the XH_2 species

ΔE_{st} for BH_2^- at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+13.63	−9.32	−2.85	−0.71	−0.11	−0.06	[+0.57]
aug-cc-pVTZ	+13.87	−10.61	−2.06	−0.75	−0.08	[−0.06]	[+0.30]
aug-cc-pVQZ	+13.93	−11.20	−1.64	−0.77	[−0.08]	[−0.06]	[+0.17]
aug-cc-pV5Z	+14.03	−11.65	−1.31	−0.79	[−0.08]	[−0.06]	[+0.13]
CBS LIMIT	[+14.11]	[−12.12]	[−0.97]	[−0.81]	[−0.08]	[−0.06]	[+0.06]
$\Delta E_{ST} = 0.06 + -0.58 + 0.20 + 0.01 + 0.00 =$ **-0.30**							

ΔE_{st} for BH_2^- at the CCSD(T)/aug-cc-pVQZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+13.63	−9.32	−2.84	−0.71	−0.11	−0.06	[+0.58]
aug-cc-pVTZ	+13.87	−10.61	−2.05	−0.76	−0.08	[−0.06]	[+0.30]
aug-cc-pVQZ	+13.93	−11.21	−1.63	−0.77	[−0.08]	[−0.06]	[+0.17]
aug-cc-pV5Z	+14.03	−11.66	−1.30	−0.79	[−0.08]	[−0.06]	[+0.13]
CBS LIMIT	[+14.11]	[−12.14]	[−0.95]	[−0.81]	[−0.08]	[−0.06]	[+0.06]
$\Delta E_{ST} = 0.06 + -0.57 + 0.22 + -0.02 + 0.07 =$ **-0.23**							

ΔE_{st} for CH_2 at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+24.21	−8.62	−4.33	−0.76	−0.19	−0.06	[+10.24]
aug-cc-pVTZ	+24.65	−10.16	−3.91	−0.88	−0.19	[−0.06]	[+9.44]
aug-cc-pVQZ	+24.70	−10.76	−3.62	−0.90	[−0.19]	[−0.06]	[+9.16]
aug-cc-pV5Z	+24.72	−11.04	−3.46	−0.91	[−0.19]	[−0.06]	[+9.05]
CBS LIMIT	[+24.72]	[−11.33]	[−3.29]	[−0.92]	[−0.19]	[−0.06]	[+8.92]
$\Delta E_{ST} = 8.92 + -0.42 + 0.38 + -0.06 + 0.13 =$ **8.95**							

ΔE_{st} for CH_2 at the CCSD(T)/aug-cc-pVQZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+24.19	−8.61	−4.33	−0.76	−0.20	−0.06	[+10.24]
aug-cc-pVTZ	+24.63	−10.14	−3.91	−0.88	−0.19	[−0.06]	[+9.44]
aug-cc-pVQZ	+24.68	−10.74	−3.62	−0.90	[−0.19]	[−0.06]	[+9.16]
aug-cc-pV5Z	+24.70	−11.02	−3.46	−0.91	[−0.19]	[−0.06]	[+9.05]
CBS LIMIT	[+24.70]	[−11.31]	[−3.29]	[−0.92]	[−0.19]	[−0.06]	[+8.92]
$\Delta E_{ST} = 8.92 + -0.41 + 0.41 + -0.06 + 0.13 =$ **8.99**							

ΔE_{st} for NH_2^+ at the CCSD(T)/aug-cc-pVTZ geometry								
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	$+\delta$ CCSDTQ	NET
aug-cc-pVDZ	+44.23	−7.58	−4.67	−0.85	−0.27	−0.09	+0.01	[+30.78]
aug-cc-pVTZ	+44.30	−9.08	−4.63	−1.04	−0.30	[−0.09]	[+0.01]	[+29.17]
aug-cc-pVQZ	+44.33	−9.82	−4.44	−1.07	[−0.30]	[−0.09]	[+0.01]	[+28.63]
aug-cc-pV5Z	+44.35	−10.19	−4.29	−1.08	[−0.30]	[−0.09]	[+0.01]	[+28.41]
CBS LIMIT	[+44.36]	[−10.59]	[−4.13]	[−1.10]	[−0.30]	[−0.09]	[+0.01]	[+28.16]
$\Delta E_{ST} = 28.16 + 0.50 + 0.43 + -0.10 + 0.15 =$ **29.14**								

ΔE_{st} for NH_2^+ at the CCSD(T)/aug-cc-pVQZ geometry								
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	$+\delta$ CCSDTQ	NET
aug-cc-pVDZ	+44.22	−7.56	−4.67	−0.85	−0.27	−0.09	+0.01	[+30.78]
aug-cc-pVTZ	+44.28	−9.06	−4.63	−1.04	−0.30	[−0.09]	[+0.01]	[+29.17]
aug-cc-pVQZ	+44.32	−9.80	−4.44	−1.07	[−0.30]	[−0.09]	[+0.01]	[+28.63]
aug-cc-pV5Z	+44.34	−10.18	−4.29	−1.08	[−0.30]	[−0.09]	[+0.01]	[+28.40]
CBS LIMIT	[+44.35]	[−10.57]	[−4.13]	[−1.10]	[−0.30]	[−0.09]	[+0.01]	[+28.16]
$\Delta E_{ST} = 28.16 + 0.51 + 0.46 + -0.10 + 0.16 =$ **29.18**								

ΔE_{st} for AlH_2^- at the CCSD(T)/aug-cc-pV(T+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	+0.46	−9.49	−3.45	−0.34	−0.01	−0.05	[−12.88]
aug-cc-pVTZ	+0.53	−10.98	−2.63	−0.40	+0.01	[−0.05]	[−13.52]
aug-cc-pVQZ	+0.65	−11.54	−2.18	−0.41	[+0.01]	[−0.05]	[−13.52]
aug-cc-pV5Z	+0.66	−11.84	−1.95	−0.42	[+0.01]	[−0.05]	[−13.57]
CBS LIMIT	[+0.66]	[−12.14]	[−1.70]	[−0.42]	[+0.01]	[−0.05]	[−13.64]
$\Delta E_{ST} = -13.64 + -0.58 + -0.42 + -0.03 + 0.02 =$ **-14.64**							

ΔE_{st} for AlH_2^- at the CCSD(T)/aug-cc-pV(Q+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	+0.46	−9.49	−3.44	−0.34	−0.01	−0.05	[−12.87]
aug-cc-pVTZ	+0.53	−10.99	−2.63	−0.40	+0.01	[−0.05]	[−13.52]
aug-cc-pVQZ	+0.65	−11.55	−2.17	−0.41	[+0.01]	[−0.05]	[−13.52]
aug-cc-pV5Z	+0.66	−11.84	−1.94	−0.42	[+0.01]	[−0.05]	[−13.58]
CBS LIMIT	[+0.66]	[−12.15]	[−1.70]	[−0.42]	[+0.01]	[−0.05]	[−13.65]
$\Delta E_{ST} = -13.65 + -0.57 + -0.42 + -0.03 + 0.02 =$ **-14.64**							

ΔE_{st} for SiH_2 at the CCSD(T)/aug-cc-pV(T+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−5.54	−9.71	−3.88	−0.29	+0.00	−0.04	[−19.45]
aug-cc-pVTZ	−5.46	−11.33	−3.15	−0.34	+0.02	[−0.04]	[−20.30]
aug-cc-pVQZ	−5.27	−12.02	−2.70	−0.35	[+0.02]	[−0.04]	[−20.36]
aug-cc-pV5Z	−5.30	−12.33	−2.46	−0.35	[+0.02]	[−0.04]	[−20.46]
CBS LIMIT	[−5.32]	[−12.65]	[−2.22]	[−0.35]	[+0.02]	[−0.04]	[−20.56]
$\Delta E_{ST} = -20.56 + -0.26 + -0.43 + -0.32 + 0.05 =$ **-21.52**							

ΔE_{st} for SiH_2 at the CCSD(T)/aug-cc-pV(Q+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−5.53	−9.71	−3.88	−0.28	+0.00	−0.04	[−19.45]
aug-cc-pVTZ	−5.45	−11.33	−3.15	−0.34	+0.02	[−0.04]	[−20.30]
aug-cc-pVQZ	−5.27	−12.02	−2.70	−0.35	[+0.02]	[−0.04]	[−20.36]
aug-cc-pV5Z	−5.30	−12.33	−2.46	−0.35	[+0.02]	[−0.04]	[−20.46]
CBS LIMIT	[−5.32]	[−12.65]	[−2.22]	[−0.35]	[+0.02]	[−0.04]	[−20.56]
$\Delta E_{ST} = -20.56 + -0.27 + -0.41 + -0.32 + 0.05 =$ **-21.51**							

ΔE_{st} for PH_2^+ at the CCSD(T)/aug-cc-pV(T+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pV(D+d)Z	−2.82	−9.28	−4.10	−0.22	+0.02	−0.05	[−16.43]
aug-cc-pV(T+d)Z	−2.69	−11.14	−3.57	−0.28	+0.03	[−0.05]	[−17.69]
aug-cc-pV(Q+d)Z	−2.61	−11.87	−3.18	−0.27	[+0.03]	[−0.05]	[−17.95]
aug-cc-pV(5+d)Z	−2.65	−12.20	−2.96	−0.28	[+0.03]	[−0.05]	[−18.10]
CBS LIMIT	[−2.68]	[−12.54]	[−2.72]	[−0.28]	[+0.03]	[−0.05]	[−18.24]
$\Delta E_{ST} = -18.24 + 0.17 + -0.26 + -0.42 + 0.07 =$ **-18.68**							

ΔE_{st} for PH_2^+ at the CCSD(T)/aug-cc-pV(Q+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pV(D+d)Z	−2.81	−9.28	−4.10	−0.22	+0.02	−0.05	[−16.43]
aug-cc-pV(T+d)Z	−2.69	−11.14	−3.57	−0.28	+0.03	[−0.05]	[−17.69]
aug-cc-pV(Q+d)Z	−2.60	−11.88	−3.18	−0.28	[+0.03]	[−0.05]	[−17.95]
aug-cc-pV(5+d)Z	−2.65	−12.20	−2.96	−0.28	[+0.03]	[−0.05]	[−18.10]
CBS LIMIT	[−2.68]	[−12.54]	[−2.72]	[−0.28]	[+0.03]	[−0.05]	[−18.24]
$\Delta E_{ST} = -18.24 + 0.16 + -0.23 + -0.42 + 0.07 =$ **-18.65**							

ΔE_{st} for GaH_2^- at the CCSD(T)/aug-cc-pwCVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−3.37	−9.94	−1.57	−0.61	+0.05	−0.13	[−15.57]
aug-cc-pVTZ	−3.61	−11.37	−0.58	−0.79	+0.09	[−0.13]	[−16.38]
aug-cc-pVQZ	−3.29	−12.06	−0.13	−0.85	[+0.09]	[−0.13]	[−16.37]
aug-cc-pV5Z	−3.28	−12.32	+0.06	−0.87	[+0.09]	[−0.13]	[−16.45]
CBS LIMIT	[−3.29]	[−12.59]	[+0.27]	[−0.89]	[+0.09]	[−0.13]	[−16.53]
$\Delta E_{ST} = -16.53 + -0.91 + -0.09 + -1.08 + 0.03 =$ **-18.59**							

ΔE_{st} for GaH_2^- at the CCSD(T)/aug-cc-pwCVQZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−3.37	−9.95	−1.56	−0.61	+0.05	−0.13	[−15.57]
aug-cc-pVTZ	−3.60	−11.38	−0.57	−0.79	+0.09	[−0.13]	[−16.38]
aug-cc-pVQZ	−3.29	−12.08	−0.12	−0.85	[+0.09]	[−0.13]	[−16.37]
aug-cc-pV5Z	−3.28	−12.33	+0.07	−0.87	[+0.09]	[−0.13]	[−16.45]
CBS LIMIT	[−3.28]	[−12.60]	[+0.27]	[−0.89]	[+0.09]	[−0.13]	[−16.53]
$\Delta E_{ST} = -16.53 + -0.87 + -0.14 + -1.08 + 0.03 =$ **-18.59**							

ΔE_{st} for GeH_2 at the CCSD(T)/aug-cc-pwCVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−10.77	−9.75	−1.83	−0.54	+0.06	−0.08	[−22.92]
aug-cc-pVTZ	−10.63	−11.42	−0.85	−0.72	+0.09	[−0.08]	[−23.63]
aug-cc-pVQZ	−10.61	−11.98	−0.44	−0.77	[+0.09]	[−0.08]	[−23.80]
aug-cc-pV5Z	−10.61	−12.23	−0.26	−0.78	[+0.09]	[−0.08]	[−23.88]
CBS LIMIT	[−10.61]	[−12.49]	[−0.07]	[−0.79]	[+0.09]	[−0.08]	[−23.96]
$\Delta E_{ST} = -23.96 + -0.35 + -0.24 + -1.68 + 0.05 =$ **-26.18**							

ΔE_{st} for GeH_2 at the CCSD(T)/aug-cc-pwCVQZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−10.77	−9.76	−1.83	−0.54	+0.06	−0.08	[−22.92]
aug-cc-pVTZ	−10.63	−11.43	−0.85	−0.72	+0.09	[−0.08]	[−23.63]
aug-cc-pVQZ	−10.61	−11.98	−0.44	−0.77	[+0.09]	[−0.08]	[−23.80]
aug-cc-pV5Z	−10.60	−12.24	−0.26	−0.78	[+0.09]	[−0.08]	[−23.88]
CBS LIMIT	[−10.60]	[−12.50]	[−0.07]	[−0.79]	[+0.09]	[−0.08]	[−23.96]
$\Delta E_{ST} = -23.96 + -0.35 + -0.26 + -1.68 + 0.05 =$ **-26.20**							

ΔE_{st} for AsH_2^+ at the CCSD(T)/aug-cc-pwCVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pwCVDZ	−9.37	−8.93	−2.20	−0.46	+0.07	−0.07	[−20.96]
aug-cc-pwCVTZ	−9.17	−10.81	−1.40	−0.62	+0.08	[−0.07]	[−21.98]
aug-cc-pwCVQZ	−9.16	−11.35	−1.03	−0.66	[+0.08]	[−0.07]	[−22.19]
aug-cc-pwCV5Z	−9.16	−11.61	−0.86	−0.67	[+0.08]	[−0.07]	[−22.28]
CBS LIMIT	[−9.16]	[−11.88]	[−0.68]	[−0.68]	[+0.08]	[−0.07]	[−22.38]
$\Delta E_{ST} = -22.38 + 0.16 + -0.34 + -1.84 + 0.06 =$ **-24.33**							

ΔE_{st} for AsH_2^+ at the CCSD(T)/aug-cc-pwCVQZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pwCVDZ	−9.37	−8.93	−2.20	−0.46	+0.07	−0.07	[−20.96]
aug-cc-pwCVTZ	−9.17	−10.81	−1.40	−0.62	+0.08	[−0.07]	[−21.98]
aug-cc-pwCVQZ	−9.16	−11.35	−1.03	−0.66	[+0.08]	[−0.07]	[−22.19]
aug-cc-pwCV5Z	−9.16	−11.61	−0.86	−0.67	[+0.08]	[−0.07]	[−22.28]
CBS LIMIT	[−9.16]	[−11.88]	[−0.68]	[−0.68]	[+0.08]	[−0.07]	[−22.38]
$\Delta E_{ST} = -22.38 + 0.15 + -0.28 + -1.84 + 0.06 =$ **-24.28**							

8 $\Delta E_{interaction}$ for isodesmic substitution reactions

ΔE_{int} for singlet X=B$^-$ species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+4.15	−2.87	+0.97	−0.82	−0.04	−0.22	[+1.17]
aug-cc-pVTZ	+4.22	−2.94	+0.98	−0.92	−0.03	[−0.22]	[+1.08]
aug-cc-pVQZ	+4.24	−3.00	+0.96	−0.94	[−0.03]	[−0.22]	[+1.00]
aug-cc-pV5Z	+4.26	−3.03	+0.95	−0.95	[−0.03]	[−0.22]	[+0.98]
CBS LIMIT	[+4.27]	[−3.05]	[+0.94]	[−0.95]	[−0.03]	[−0.22]	[+0.95]
$\Delta E_{ST} = 0.95 + -0.01 + -0.01 + -0.00 + -0.04 =$ **0.89**							

ΔE_{int} for triplet X=B$^-$ species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+4.45	−6.35	+0.90	−0.60	−0.02	−0.10	[−1.73]
aug-cc-pVTZ	+4.59	−6.98	+1.07	−0.75	−0.00	[−0.10]	[−2.17]
aug-cc-pVQZ	+4.65	−7.27	+1.17	−0.78	[−0.00]	[−0.10]	[−2.34]
aug-cc-pV5Z	+4.76	−7.57	+1.34	−0.80	[−0.00]	[−0.10]	[−2.37]
CBS LIMIT	[+4.85]	[−7.88]	[+1.53]	[−0.82]	[−0.00]	[−0.10]	[−2.43]
$\Delta E_{ST} = -2.43 + -0.25 + -0.15 + 0.05 + -0.10 =$ **-2.88**							

difference between zpve in carbene??

ΔE_{int} for singlet X=C species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	−5.25	−4.40	+1.34	−2.02	−0.23	−0.44	[−11.01]
aug-cc-pVTZ	−5.65	−4.57	+1.40	−2.19	−0.21	[−0.44]	[−11.65]
aug-cc-pVQZ	−5.73	−4.65	+1.39	−2.23	[−0.21]	[−0.44]	[−11.85]
aug-cc-pV5Z	−5.75	−4.67	+1.39	−2.24	[−0.21]	[−0.44]	[−11.92]
CBS LIMIT	[−5.76]	[−4.70]	[+1.39]	[−2.26]	[−0.21]	[−0.44]	[−11.97]
$\Delta E_{ST} = -11.97 + 0.58 + -0.05 + -0.01 + -0.01 =$ **-11.46**							

ΔE_{int} for triplet X=C species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+4.84	−14.19	−0.75	−1.65	−0.26	−0.31	[−12.31]
aug-cc-pVTZ	+4.29	−14.95	−0.55	−1.95	−0.21	[−0.31]	[−13.69]
aug-cc-pVQZ	+4.22	−15.21	−0.47	−2.03	[−0.21]	[−0.31]	[−14.02]
aug-cc-pV5Z	+4.20	−15.29	−0.42	−2.06	[−0.21]	[−0.31]	[−14.10]
CBS LIMIT	[+4.19]	[−15.37]	[−0.38]	[−2.09]	[−0.21]	[−0.31]	[−14.17]
$\Delta E_{ST} = -14.17 + -0.06 + -0.10 + -0.00 + 0.02 =$ **-14.32**							

ΔE_{int} for singlet X=N^+ species at the CCSD(T)/aug-cc-pVTZ geometry								
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	+δ CCSDTQ	NET
aug-cc-pVDZ	−50.74	−8.06	−0.96	−4.35	−0.46	−0.89	+0.16	[−65.30]
aug-cc-pVTZ	−51.08	−8.05	−0.71	−4.62	−0.40	[−0.89]	[+0.16]	[−65.58]
aug-cc-pVQZ	−51.18	−8.13	−0.74	−4.69	[−0.40]	[−0.89]	[+0.16]	[−65.86]
aug-cc-pV5Z	−51.20	−8.15	−0.74	−4.72	[−0.40]	[−0.89]	[+0.16]	[−65.93]
CBS LIMIT	[−51.21]	[−8.16]	[−0.75]	[−4.74]	[−0.40]	[−0.89]	[+0.16]	[−65.99]
$\Delta E_{ST} = -65.99 + 1.46 + -0.04 + 0.02 + 0.03 =$ **-64.53**								

ΔE_{int} for triplet X=N^+ species at the CCSD(T)/aug-cc-pVTZ geometry								
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	+δ CCSDTQ	NET
aug-cc-pVDZ	−49.82	−1.78	−4.96	−0.61	−0.53	+0.11	−0.08	[−57.67]
aug-cc-pVTZ	−51.00	−1.99	−4.99	−0.82	−0.55	[+0.11]	[−0.08]	[−59.33]
aug-cc-pVQZ	−51.09	−2.33	−5.04	−0.88	[−0.55]	[+0.11]	[−0.08]	[−59.86]
aug-cc-pV5Z	−51.11	−2.43	−5.03	−0.90	[−0.55]	[+0.11]	[−0.08]	[−60.00]
CBS LIMIT	[−51.12]	[−2.54]	[−5.03]	[−0.92]	[−0.55]	[+0.11]	[−0.08]	[−60.13]
$\Delta E_{ST} = -60.13 + 2.11 + -0.01 + -0.00 + -0.01 =$ **-58.04**								

ΔE_{int} for singlet X=Al^- species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+0.28	−1.57	+0.37	−0.32	+0.05	−0.07	[−1.25]
aug-cc-pVTZ	+0.44	−1.49	+0.49	−0.32	+0.07	[−0.07]	[−0.88]
aug-cc-pVQZ	+0.46	−1.43	+0.47	−0.33	[+0.07]	[−0.07]	[−0.82]
aug-cc-pV5Z	+0.46	−1.45	+0.47	−0.33	[+0.07]	[−0.07]	[−0.83]
CBS LIMIT	[+0.46]	[−1.46]	[+0.47]	[−0.33]	[+0.07]	[−0.07]	[−0.85]
$\Delta E_{ST} = -0.85 + 0.21 + -0.07 + -0.04 + -0.02 =$ **-0.77**							

ΔE_{int} for triplet X=Al^- species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	+6.32	−1.56	+0.50	−0.26	+0.02	−0.05	[+4.96]
aug-cc-pVTZ	+6.26	−1.61	+0.56	−0.30	+0.03	[−0.05]	[+4.89]
aug-cc-pVQZ	+6.25	−1.64	+0.55	−0.31	[+0.03]	[−0.05]	[+4.83]
aug-cc-pV5Z	+6.25	−1.66	+0.55	−0.31	[+0.03]	[−0.05]	[+4.80]
CBS LIMIT	[+6.25]	[−1.69]	[+0.55]	[−0.32]	[+0.03]	[−0.05]	[+4.76]
$\Delta E_{ST} = 4.76 + 0.07 + 0.05 + 0.16 + -0.01 =$ **5.02**							

ΔE_{int} for singlet X=Si species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	+δ MP2	+δ CCSD	+δ CCSD(T)	+δ CCSDT	+δ CCSDT(Q)	NET
aug-cc-pVDZ	−2.86	−1.56	+0.73	−0.57	+0.02	−0.10	[−4.35]
aug-cc-pVTZ	−2.85	−1.47	+0.85	−0.59	+0.05	[−0.10]	[−4.12]
aug-cc-pVQZ	−2.86	−1.42	+0.83	−0.61	[+0.05]	[−0.10]	[−4.11]
aug-cc-pV5Z	−2.86	−1.43	+0.82	−0.61	[+0.05]	[−0.10]	[−4.14]
CBS LIMIT	[−2.86]	[−1.44]	[+0.82]	[−0.62]	[+0.05]	[−0.10]	[−4.16]
$\Delta E_{ST} = -4.16 + 0.50 + -0.03 + -0.05 + -0.02 =$ **-3.76**							

ΔE_{int} for triplet X=Si species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	+3.18	−1.84	+0.31	−0.43	−0.04	−0.08	[+1.11]
aug-cc-pVTZ	+3.10	−1.81	+0.40	−0.48	−0.02	[−0.08]	[+1.10]
aug-cc-pVQZ	+3.04	−1.83	+0.38	−0.50	[−0.02]	[−0.08]	[+1.00]
aug-cc-pV5Z	+3.03	−1.85	+0.38	−0.51	[−0.02]	[−0.08]	[+0.95]
CBS LIMIT	[+3.03]	[−1.88]	[+0.38]	[−0.51]	[−0.02]	[−0.08]	[+0.92]
$\Delta E_{ST} = 0.92 + 0.41 + 0.01 + 0.02 + -0.00 =$ **1.36**							

ΔE_{int} for singlet X=P^+ species at the CCSD(T)/aug-cc-pV(T+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−9.33	−2.72	+0.69	−2.04	−0.10	−0.33	[−13.83]
aug-cc-pVTZ	−9.19	−2.60	+0.88	−2.12	−0.06	[−0.33]	[−13.44]
aug-cc-pVQZ	−9.17	−2.59	+0.86	−2.16	[−0.06]	[−0.33]	[−13.45]
aug-cc-pV5Z	−9.16	−2.58	+0.85	−2.17	[−0.06]	[−0.33]	[−13.45]
CBS LIMIT	[−9.15]	[−2.57]	[+0.85]	[−2.18]	[−0.06]	[−0.33]	[−13.45]
$\Delta E_{ST} = -13.45 + 0.57 + -0.00 + -0.04 + -0.01 =$ **-12.94**							

ΔE_{int} for triplet X=P^+ species at the CCSD(T)/aug-cc-pV(T+d)Z geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	+3.16	−5.85	−0.32	−1.60	−0.22	−0.30	[−5.12]
aug-cc-pVTZ	+3.21	−5.84	−0.15	−1.79	−0.20	[−0.30]	[−5.06]
aug-cc-pVQZ	+3.20	−5.92	−0.13	−1.84	[−0.20]	[−0.30]	[−5.18]
aug-cc-pV5Z	+3.20	−5.94	−0.12	−1.86	[−0.20]	[−0.30]	[−5.21]
CBS LIMIT	[+3.20]	[−5.97]	[−0.10]	[−1.88]	[−0.20]	[−0.30]	[−5.24]
$\Delta E_{ST} = -5.24 + 0.38 + -0.00 + -0.02 + 0.00 =$ **-4.88**							

ΔE_{int} for singlet X=Ga^- species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−1.52	−1.75	+0.52	−0.28	+0.02	−0.04	[−3.05]
aug-cc-pVTZ	−1.30	−1.67	+0.64	−0.29	+0.04	[−0.04]	[−2.64]
aug-cc-pVQZ	−1.30	−1.62	+0.64	−0.30	[+0.04]	[−0.04]	[−2.58]
aug-cc-pV5Z	−1.29	−1.63	+0.64	−0.30	[+0.04]	[−0.04]	[−2.59]
CBS LIMIT	[−1.29]	[−1.63]	[+0.64]	[−0.30]	[+0.04]	[−0.04]	[−2.59]
$\Delta E_{ST} = -2.59 + 0.19 + -0.03 + -0.38 + -0.02 =$ **-2.82**							

ΔE_{int} for triplet X=Ga^- species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	+7.25	−2.08	+0.50	−0.26	+0.01	−0.04	[+5.38]
aug-cc-pVTZ	+7.05	−2.10	+0.59	−0.30	+0.01	[−0.04]	[+5.21]
aug-cc-pVQZ	+7.27	−2.28	+0.62	−0.32	[+0.01]	[−0.04]	[+5.26]
aug-cc-pV5Z	+7.27	−2.33	+0.63	−0.33	[+0.01]	[−0.04]	[+5.21]
CBS LIMIT	[+7.27]	[−2.39]	[+0.65]	[−0.34]	[+0.01]	[−0.04]	[+5.16]
$\Delta E_{ST} = 5.16 + -0.02 + -0.02 + 0.23 + -0.01 =$ **5.35**							

ΔE_{int} for singlet X=Ge species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−4.22	−1.83	+0.84	−0.48	+0.01	−0.09	[−5.77]
aug-cc-pVTZ	−4.08	−1.76	+0.94	−0.50	+0.03	[−0.09]	[−5.46]
aug-cc-pVQZ	−4.09	−1.70	+0.92	−0.50	[+0.03]	[−0.09]	[−5.43]
aug-cc-pV5Z	−4.09	−1.70	+0.91	−0.51	[+0.03]	[−0.09]	[−5.44]
CBS LIMIT	[−4.09]	[−1.70]	[+0.91]	[−0.51]	[+0.03]	[−0.09]	[−5.44]
$\Delta E_{ST} = -5.44 + 0.47 + 0.02 + -0.36 + -0.02 =$ **-5.33**							

ΔE_{int} for triplet X=Ge species at the CCSD(T)/aug-cc-pVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	+3.79	−1.87	+0.18	−0.42	−0.03	−0.07	[+1.58]
aug-cc-pVTZ	+3.77	−1.84	+0.28	−0.47	−0.02	[−0.07]	[+1.64]
aug-cc-pVQZ	+3.75	−1.85	+0.27	−0.48	[−0.02]	[−0.07]	[+1.59]
aug-cc-pV5Z	+3.74	−1.87	+0.27	−0.49	[−0.02]	[−0.07]	[+1.56]
CBS LIMIT	[+3.75]	[−1.89]	[+0.27]	[−0.50]	[−0.02]	[−0.07]	[+1.54]
$\Delta E_{ST} = 1.54 + 0.35 + 0.04 + 0.05 + 0.00 =$ **1.97**							

ΔE_{int} for singlet X=As^+ species at the CCSD(T)/aug-cc-pwCVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	−7.93	−3.52	+1.32	−1.62	−0.04	−0.30	[−12.11]
aug-cc-pVTZ	−7.71	−3.47	+1.43	−1.69	−0.02	[−0.30]	[−11.76]
aug-cc-pVQZ	−7.69	−3.43	+1.42	−1.71	[−0.02]	[−0.30]	[−11.74]
aug-cc-pV5Z	−7.69	−3.42	+1.41	−1.72	[−0.02]	[−0.30]	[−11.74]
CBS LIMIT	[−7.69]	[−3.40]	[+1.40]	[−1.73]	[−0.02]	[−0.30]	[−11.74]
$\Delta E_{ST} = -11.74 + 0.55 + 0.06 + -0.38 + -0.01 =$ **-11.52**							

ΔE_{int} for triplet X=As^+ species at the CCSD(T)/aug-cc-pwCVTZ geometry							
	SCF	$+\delta$ MP2	$+\delta$ CCSD	$+\delta$ CCSD(T)	$+\delta$ CCSDT	$+\delta$ CCSDT(Q)	NET
aug-cc-pVDZ	+3.95	−4.89	−0.17	−1.38	−0.18	−0.25	[−2.92]
aug-cc-pVTZ	+4.08	−4.93	−0.03	−1.55	−0.18	[−0.25]	[−2.86]
aug-cc-pVQZ	+4.07	−4.95	−0.00	−1.59	[−0.18]	[−0.25]	[−2.90]
aug-cc-pV5Z	+4.07	−4.96	+0.01	−1.60	[−0.18]	[−0.25]	[−2.91]
CBS LIMIT	[+4.08]	[−4.97]	[+0.02]	[−1.62]	[−0.18]	[−0.25]	[−2.92]
$\Delta E_{ST} = -2.92 + 0.36 + 0.05 + -0.24 + 0.00 =$ **-2.74**							

9 Frequencies of HXCN species at the CCSD(T)/QZ level of theory

State	a'	a'	a'	a'	a'	a''
			HBCN$^-$			
^{1}A$'$	2383.28	2069.52	884.86	759.05	399.96	318.30
X^{3}A$''$	2608.80	1985.23	925.13	701.16	384.47	443.45
			HCCN			
^{1}A$'$	3058.40	2058.12	1055.85	972.04	426.33	292.08
X^{3}A$''$	3345.20	1811.32	1160.90	559.34	384.96	425.64
			HNCN$^+$			
^{1}A$'$	3347.98	1923.25	1210.95	909.93	439.69	267.58
X^{3}A$''$	3578.67 (σ^+)	1935.98 (σ^+)	1003.81 (σ^+)	472.89 (π)	387.99 (π)	
			HAlCN$^-$			
X^{1}A$'$	2137.22	1573.94	667.93	387.73	239.14	203.50
^{3}A$''$	2124.85	1799.90	568.88	475.38	249.80	232.53
			HSiCN			
X^{1}A$'$	2176.70	2100.45	831.56	562.70	259.63	206.22
^{3}A$''$	2240.78	2154.13	697.87	621.33	252.30	303.78
			HPCN$^+$			
X^{1}A$'$	2387.76	2109.20	920.12	708.10	256.26	167.09
^{3}A$''$	2360.72	2025.91	734.96	701.51	218.94	269.31
			HGaCN$^-$			
X^{1}A$'$	2130.14	1504.29	647.38	297.20	215.22	182.01
^{3}A$''$	2119.20	1837.52	561.72	393.87	248.19	291.16
			HGeCN			
X^{1}A$'$	2177.75	1971.48	760.64	445.56	236.26	189.81
^{3}A$''$	2161.37	2122.37	635.44	497.90	238.62	251.53
			HAsCN$^+$			
X^{1}A$'$	2206.89	2123.41	817.44	562.05	227.95	151.21
^{3}A$''$	2142.13	2071.02	629.55	564.73	198.67	244.92

10 Comparison of geometry parameters with previous studies

Species	State	X–H(Å)	X–C(Å)	C–N(Å)	H–X–C(°)	X–C–N(°)	Method	Reference
$HBCN^-$	$^1A'$	1.223	1.562	1.178	106.34	173.18	CCSD(T)/aug-cc-pVQZ	a
		1.225	1.567	1.181	106.19	173.04	CCSD(T)/aug-cc-pVTZ	a
		1.235	1.586	1.203	106.2	171.0	MBPT(2)/DZP(d)	*Int. J. Quant. Chem.* **84**, 140 (2001)
	X^3A'	1.194	1.493	1.186	131.70	176.39	CCSD(T)/aug-cc-pVQZ	a
		1.195	1.496	1.189	131.76	176.28	CCSD(T)/aug-cc-pVTZ	a
		1.203	1.552	1.168	124.6	178.4	MBPT(2)/DZP(d)	*Int. J. Quant. Chem.* **84**, 140 (2001)
HCCN	$^1A'$	1.099	1.392	1.179	109.34	172.26	CCSD(T)/aug-cc-pVQZ	a
		1.100	1.395	1.182	109.11	172.07	CCSD(T)/aug-cc-pVTZ	a
		1.096	1.386	1.175	109.66	172.41	RCCSD(T)/CBS + core + rel	*J. Chem. Phys.* **135**, 244310 (2011)
		1.106	1.419	1.198	107.4	101.6	QCISD(T)/D95**	*Chem. Phys. Lett.* **202**, 33 (1993)
		1.10	1.24	1.18	111.5	171.0	B3LYP/6-311++G**	*J. Mol. Struct. THEOCHEM* **728**, 15 (2005)
		1.10	1.23	1.18	108.5	171.8	MP3/6-311G*	*J. Mol. Struct. THEOCHEM* **728**, 15 (2005)
	X^3A'	1.071	1.325	1.193	145.94	175.15	CCSD(T)/aug-cc-pVQZ	a
		1.072	1.329	1.196	145.55	175.02	CCSD(T)/aug-cc-pVTZ	a
		1.069	1.327	1.185	144.95	175.45	RCCSD(T)/CBS + core + rel	*J. Chem. Phys.* **135**, 244310 (2011)
		1.078	1.353	1.210	140.5	174.7	QCISD(T)/D95**	*Chem. Phys. Lett.* **202**, 33 (1993)
		1.07	1.29	1.20	159.3	176.5	B3LYP/6-311++G**	*J. Mol. Struct. THEOCHEM* **728**, 15 (2005)
		1.08	1.38	1.14	134.8	178.3	MP3/6-311G*	*J. Mol. Struct. THEOCHEM* **728**, 15 (2005)
		1.071	1.331	1.188	144.56	175.33	CCSD(T)/cc-pV5Z	*J. Phys. Chem. A* **106**, 6183 (2002)
$HNCN^+$	$^1A'$	1.035	1.250	1.223	118.94	171.28	CCSD(T)/aug-cc-pVQZ	a
		1.037	1.254	1.226	118.52	171.16	CCSD(T)/aug-cc-pVTZ	a
		1.021	1.277	1.209	116.2	167.9	CASSCF(8,8)/6-31G(d)	*Chem. Phys. Chem.* **5**, 1345 (2004)
	X^3A'	1.017	1.164	1.306	180.00	180.00	CCSD(T)/aug-cc-pVQZ	a
		1.018	1.167	1.310	180.00	180.00	CCSD(T)/aug-cc-pVTZ	a
		1.006	1.158	1.338	179.2	180.0	CASSCF(8,8)/6-31G(d)	*Chem. Phys. Chem.* **5**, 1345 (2004)
		1.016	1.164	1.303	180.0	180.0	CCSD(T)/CBS	*J. Chem. Phys.* **122**, 064316 (2005)
$HAlCN^-$	X^1A'	1.669	2.086	1.172	92.14	173.82	CCSD(T)/aug-cc-pV(Q+d)Z	a
		1.673	2.093	1.175	92.07	173.90	CCSD(T)/aug-cc-pV(T+d)Z	a
	$^3A'$	1.607	1.992	1.172	114.18	177.65	CCSD(T)/aug-cc-pV(Q+d)Z	a
		1.609	1.997	1.176	114.24	177.65	CCSD(T)/aug-cc-pV(T+d)Z	a
HSiCN	X^1A'	1.511	1.878	1.167	92.13	174.00	CCSD(T)/aug-cc-pV(Q+d)Z	a
		1.513	1.884	1.171	92.06	174.14	CCSD(T)/aug-cc-pV(T+d)Z	a
		1.521	1.877	1.161	91.8	173.1	B3LYP/6-311G**	*Chem. Phys.* **313**, 1 (2005)
		1.510	1.886	1.169	92.04	174.24	QCISD/6-311G(d,p)	*Chem. Phys.* **323**, 413 (2006)
		1.515	1.886	1.166	92.2	172.2	ACPF/aug-cc-pVTZ	*J. Phys. Chem. A* **109**, 11437 (2005)
		1.534	1.887	1.169	94.3	175.5	CASSCF($14e^-$,13o)/aug-cc-pVTZ	*Theo. Chem. Acc.* **124**, 85 (2009)
	$^3A'$	1.477	1.818	1.168	116.30	177.01	CCSD(T)/aug-cc-pV(Q+d)Z	a
		1.479	1.823	1.172	116.47	177.01	CCSD(T)/aug-cc-pV(T+d)Z	a
		1.484	1.809	1.164	117.1	176.1	B3LYP/6-311G**	*Chem. Phys.* **313**, 1 (2005)
		1.473	1.822	1.172	116.46	176.54	QCISD/6-311G(d,p)	*Chem. Phys.* **323**, 413 (2006)
		1.478	1.827	1.166	116.7	177.1	ACPF/aug-cc-pVTZ	*J. Phys. Chem. A* **109**, 11437 (2005)
		1.469	1.854	1.169	116.1	177.9	CASSCF($14e^-$,13o)/aug-cc-pVTZ	*Theo. Chem. Acc.* **124**, 85 (2009)
$HPCN^+$	X^1A'	1.424	1.720	1.179	93.89	174.05	CCSD(T)/aug-cc-pV(Q+d)Z	a
		1.425	1.724	1.182	93.83	174.14	CCSD(T)/aug-cc-pV(T+d)Z	a
		1.431	1.720	1.168	93.419	174.213	B3LYP/6-311++G(2df, p)	*J. Theor. Comput. Chem* **9**, 189 (2010)
	$^3A'$	1.418	1.691	1.180	117.86	175.13	CCSD(T)/aug-cc-pV(Q+d)Z	a
		1.419	1.696	1.184	118.00	175.09	CCSD(T)/aug-cc-pV(T+d)Z	a
		1.427	1.685	1.176	115.091	175.021	B3LYP/6-311++G(2df, p)	*J. Theor. Comput. Chem* **9**, 189 (2010)
$HGaCN^-$	X^1A'	1.675	2.138	1.172	91.45	172.51	CCSD(T)/aug-cc-pwCVQZ	a
		1.677	2.144	1.174	91.37	172.78	CCSD(T)/aug-cc-pwCVTZ	a
	$^3A'$	1.578	1.987	1.172	116.29	176.70	CCSD(T)/aug-cc-pwCVQZ	a
		1.579	1.991	1.174	116.25	176.85	CCSD(T)/aug-cc-pwCVTZ	a
HGeCN	X^1A'	1.575	1.967	1.167	91.32	174.11	CCSD(T)/aug-cc-pwCVQZ	a
		1.576	1.970	1.169	91.30	174.32	CCSD(T)/aug-cc-pwCVTZ	a
		1.48	1.79	1.17	179.9	180.0	B3LYP/6-311++G**	*J. Organomet. Chem.* **690**, 4692 (2005)
		1.65	2.09	1.19	129.8	121.3	MP2/6-311++G**	*J. Organomet. Chem.* **690**, 4692 (2005)
	$^3A'$	1.525	1.888	1.167	116.96	176.75	CCSD(T)/aug-cc-pwCVQZ	a
		1.525	1.891	1.169	116.98	176.84	CCSD(T)/aug-cc-pwCVTZ	a
		1.54	1.90	1.16	116.8	176.2	B3LYP/6-311++G**	*J. Organomet. Chem.* **690**, 4692 (2005)
		1.53	1.95	1.14	115.1	175.5	MP2/6-311++G**	*J. Organomet. Chem.* **690**, 4692 (2005)
$HAsCN^+$	X^1A'	1.522	1.843	1.175	92.56	174.62	CCSD(T)/aug-cc-pwCVQZ	a
		1.523	1.846	1.177	92.52	174.84	CCSD(T)/aug-cc-pwCVTZ	a
	$^3A'$	1.512	1.812	1.176	117.18	176.07	CCSD(T)/aug-cc-pwCVQZ	a
		1.513	1.815	1.178	117.15	176.19	CCSD(T)/aug-cc-pwCVTZ	a

a. This work

11 Geometry coordinates for the XH_4 species

Singlet BH_4^- at CCSD(T)/aug-cc-pVTZ in bohr			
B	-0.00000279	0.00000000	-0.00000000
H	2.34259499	0.00000000	-0.00000000
H	-0.78085482	1.10431364	-1.91272734
H	-0.78085482	-2.20862729	0.00000000
H	-0.78085482	1.10431364	1.91272734

Singlet CH_4 at CCSD(T)/aug-cc-pVTZ in bohr			
C	-0.00000000	-0.00000000	0.00000000
H	0.00000000	-1.68167833	1.18912615
H	-0.00000000	1.68167833	1.18912615
H	1.68167833	0.00000000	-1.18912615
H	-1.68167833	0.00000000	-1.18912615

Singlet NH_4^+ at CCSD(T)/aug-cc-pVTZ in bohr			
N	-0.00000000	-0.00000000	0.00000000
H	-1.93416570	-0.00000000	0.00000000
H	0.64472190	-0.91177445	-1.57923968
H	0.64472190	1.82354891	0.00000000
H	0.64472190	-0.91177445	1.57923968

Singlet AlH_4^- at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
Al	0.00000000	-0.00000000	-0.00000000
H	0.00000000	-2.53809191	1.79470200
H	0.00000000	2.53809191	1.79470200
H	2.53809191	-0.00000000	-1.79470200
H	-2.53809191	0.00000000	-1.79470200

Singlet SiH_4 at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
Si	-0.00000053	-0.00000000	0.00000000
H	2.79697503	-0.00000000	0.00000000
H	-0.93232008	1.31850792	-2.28372271
H	-0.93232008	-2.63701585	-0.00000000
H	-0.93232008	1.31850792	2.28372271

Singlet PH_4^+ at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
P	-0.00000000	0.00000000	-0.00000000
H	-0.00000000	-2.15153582	1.52136557
H	0.00000000	2.15153582	1.52136557
H	2.15153582	-0.00000000	-1.52136557
H	-2.15153582	-0.00000000	-1.52136557

Singlet GaH_4^- at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ga	-0.00000044	-0.00000000	0.00000000
H	3.04715043	-0.00000000	0.00000000
H	-1.01570678	1.43644257	-2.48799152
H	-1.01570678	-2.87288514	-0.00000000
H	-1.01570678	1.43644257	2.48799152

Singlet GeH_4 at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ge	0.00000000	0.00000000	-0.00000000
H	-0.00000000	-2.35024219	1.66187219
H	0.00000000	2.35024219	1.66187219
H	2.35024219	-0.00000000	-1.66187219
H	-2.35024219	-0.00000000	-1.66187219

Singlet AsH_4^+ at CCSD(T)/aug-cc-pwCVTZ in bohr			
As	0.00000000	0.00000000	-0.00000000
H	-0.00000000	-2.28359993	1.61474900
H	0.00000000	2.28359993	1.61474900
H	2.28359993	-0.00000000	-1.61474900
H	-2.28359993	-0.00000000	-1.61474900

12 Geometry coordinates for the H_3XCN species

Singlet H_3BCN^- at CCSD(T)/aug-cc-pVTZ in bohr			
B	2.68968654	-0.00000000	0.00000000
H	3.42432137	-1.09720039	-1.90040683
C	-0.34442745	0.00000000	0.00000000
N	-2.55885254	-0.00000000	-0.00000000
H	3.42432137	2.19440078	-0.00000000
H	3.42432137	-1.09720039	1.90040683

Singlet H_3CCN at CCSD(T)/aug-cc-pVTZ in bohr			
C	2.45395662	0.00000000	0.00000000
H	3.15132249	-0.96901908	-1.67839028
C	-0.31627392	0.00000000	0.00000000
N	-2.51231533	-0.00000000	-0.00000000
H	3.15132249	1.93803816	-0.00000000
H	3.15132249	-0.96901908	1.67839028

Singlet H_3NCN^+ at CCSD(T)/aug-cc-pVTZ in bohr			
N	2.28109168	0.00000000	0.00000000
H	2.96336462	-0.91256072	-1.58060154
C	-0.39199917	0.00000000	0.00000000
N	-2.58500131	-0.00000000	-0.00000000
H	2.96336462	1.82512145	-0.00000000
H	2.96336462	-0.91256072	1.58060154

Singlet H_3AlCN^- at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
Al	2.29946026	0.00000000	0.00000000
H	3.17207149	-1.47062452	-2.54719638
C	-1.56200010	0.00000000	0.00000000
N	-3.77700309	-0.00000000	-0.00000000
H	3.17207149	2.94124903	-0.00000000
H	3.17207149	-1.47062452	2.54719638

Singlet H_3SiCN at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
Si	2.10047200	0.00000000	0.00000000
H	2.93679422	-1.32810978	-2.30035361
C	-1.41484953	0.00000000	0.00000000
N	-3.61819710	-0.00000000	-0.00000000
H	2.93679422	2.65621956	-0.00000000
H	2.93679422	-1.32810978	2.30035361

Singlet H_3PCN^+ at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
P	1.89793985	0.00000000	0.00000000
H	2.75789503	-1.24716103	-2.16014628
C	-1.39423898	0.00000000	0.00000000
N	-3.59877384	-0.00000000	-0.00000000
H	2.75789503	2.49432207	-0.00000000
H	2.75789503	-1.24716103	2.16014628

Singlet H_3GaCN^- at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ga	1.31586891	0.00000000	0.00000000
H	2.14712831	-1.44475814	-2.50239450
C	-2.54645682	-0.00000000	-0.00000000
N	-4.75833625	-0.00000000	-0.00000000
H	2.14712831	2.88951628	-0.00000000
H	2.14712831	-1.44475814	2.50239450

Singlet H_3GeCN at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ge	1.19371723	-0.00000000	-0.00000000
H	2.02790525	-1.37132889	-2.37521131
C	-2.44462117	0.00000000	0.00000000
N	-4.64446949	0.00000000	0.00000000
H	2.02790525	2.74265778	0.00000000
H	2.02790525	-1.37132889	2.37521131

13 Geometry coordinates for the XH_2 species

Singlet BH_2^- at CCSD(T)/aug-cc-pVTZ in bohr			
H	0.00000000	-1.86138634	1.20590575
B	0.00000000	0.00000000	-0.22078450
H	0.00000000	1.86138634	1.20590575

Singlet BH_2^- at CCSD(T)/aug-cc-pVQZ in bohr			
H	0.00000000	-1.85995411	1.20137391
B	0.00000000	-0.00000000	-0.21995479
H	0.00000000	1.85995411	1.20137391

Triplet BH_2^- at CCSD(T)/aug-cc-pVQZ in bohr			
H	0.00000000	-2.06052878	0.82458509
B	0.00000000	-0.00000000	-0.15097001
H	0.00000000	2.06052878	0.82458509

Triplet BH_2^- at CCSD(T)/aug-cc-pVQZ in bohr			
H	0.00000000	-2.05772475	0.82283260
B	0.00000000	0.00000000	-0.15064916
H	0.00000000	2.05772475	0.82283260

Singlet CH_2 at CCSD(T)/aug-cc-pVTZ in bohr			
H	0.00000000	-1.62975012	1.13235972
C	0.00000000	-0.00000000	-0.19020341
H	0.00000000	1.62975012	1.13235972

Singlet CH_2 at CCSD(T)/aug-cc-pVQZ in bohr			
H	0.00000000	-1.62845369	1.12888442
C	0.00000000	-0.00000000	-0.18961966
H	0.00000000	1.62845369	1.12888442

Triplet CH_2 at CCSD(T)/aug-cc-pVTZ in bohr			
H	0.00000000	-1.87451102	0.68746268
C	0.00000000	-0.00000000	-0.11547368
H	0.00000000	1.87451102	0.68746268

Triplet CH_2 at CCSD(T)/aug-cc-pVQZ in bohr			
H	0.00000000	-1.87218848	0.68570448
C	0.00000000	-0.00000000	-0.11517836
H	0.00000000	1.87218848	0.68570448

Singlet NH_2^+ at CCSD(T)/aug-cc-pVTZ in bohr			
H	0.00000000	-1.60224162	1.02473860
N	0.00000000	0.00000000	-0.14750436
H	0.00000000	1.60224162	1.02473860

Singlet NH_2^+ at CCSD(T)/aug-cc-pVQZ in bohr			
H	0.00000000	-1.60073114	1.02121466
N	0.00000000	0.00000000	-0.14699711
H	0.00000000	1.60073114	1.02121466

Triplet NH_2^+ at CCSD(T)/aug-cc-pVTZ in bohr			
H	0.00000000	-1.89492368	0.40835954
N	0.00000000	0.00000000	-0.05878066
H	0.00000000	1.89492368	0.40835954

Triplet NH_2^+ at CCSD(T)/aug-cc-pVQZ in bohr			
H	0.00000000	-1.89180487	0.40928641
N	-0.00000000	0.00000000	-0.05891408
H	0.00000000	1.89180487	0.40928641

Singlet AlH_2^- at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
H	0.00000000	-2.35639772	2.00242616
Al	0.00000000	0.00000000	-0.14959082
H	0.00000000	2.35639772	2.00242616

Singlet AlH_2^- at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
H	0.00000000	-2.35142435	1.99562165
AL	0.00000000	0.00000000	-0.14908249
H	0.00000000	2.35142435	1.99562165

Triplet AlH_2^- at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
H	0.00000000	-2.62764530	1.46858103
Al	0.00000000	0.00000000	-0.10971003
H	0.00000000	2.62764530	1.46858103

Triplet AlH_2^- at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
H	0.00000000	-2.62276527	1.46820838
Al	0.00000000	0.00000000	-0.10968219
H	0.00000000	2.62276527	1.46820838

Singlet SiH_2 at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
H	0.00000000	-2.06973992	1.85633956
Si	0.00000000	-0.00000000	-0.13374346
H	0.00000000	2.06973992	1.85633956

Singlet SiH_2 at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
H	0.00000000	-2.06720584	1.85264974
Si	0.00000000	0.00000000	-0.13347762
H	0.00000000	2.06720584	1.85264974

Triplet SiH_2 at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
H	-0.00000000	-2.40632714	1.33775811
Si	0.00000000	-0.00000000	-0.09638129
H	-0.00000000	2.40632714	1.33775811

Triplet SiH_2 at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
H	0.00000000	-2.40188137	1.33846159
Si	0.00000000	0.00000000	-0.09643197
H	0.00000000	2.40188137	1.33846159

Singlet PH_2^+ at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
H	0.00000000	-1.94258415	1.74334640
P	0.00000000	0.00000000	-0.11345010
H	0.00000000	1.94258415	1.74334640

Singlet PH_2^+ at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
H	0.00000000	-1.94184666	1.74113880
P	0.00000000	-0.00000000	-0.11330644
H	0.00000000	1.94184666	1.74113880

Triplet PH_2^+ at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
H	0.00000000	-2.33078339	1.21402804
P	0.00000000	0.00000000	-0.07900415
H	0.00000000	2.33078339	1.21402804

Triplet PH_2^+ at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
H	0.00000000	-2.32708011	1.21624245
P	-0.00000000	-0.00000000	-0.07914825
H	0.00000000	2.32708011	1.21624245

Singlet GaH_2^- at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ga	0.00000000	0.00000000	0.06194681
H	0.00000000	-2.33814569	-2.11828428
H	0.00000000	2.33814569	-2.11828428

Singlet GaH_2^- at CCSD(T)/aug-cc-pwCVQZ in bohr			
Ga	0.00000000	-0.00000000	0.06181393
H	0.00000000	-2.33614404	-2.11374050
H	0.00000000	2.33614404	-2.11374050

Triplet GaH_2^- at CCSD(T)/aug-cc-pwCVTZ in bohr			
GA	0.00000000	-0.00000000	0.04215048
H	0.00000000	-2.61818319	-1.44134446
H	0.00000000	2.61818319	-1.44134446

Triplet GaH_2^- at CCSD(T)/aug-cc-pwCVQZ in bohr			
Ga	0.00000000	0.00000000	0.04217200
H	0.00000000	-2.61616767	-1.44208049
H	0.00000000	2.61616767	-1.44208049

Singlet GeH_2 at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ge	0.00000000	0.00000000	0.05530950
H	0.00000000	-2.14042792	-2.02839951
H	0.00000000	2.14042792	-2.02839951

Singlet GeH_2 at CCSD(T)/aug-cc-pwCVQZ in bohr			
Ge	0.00000000	0.00000000	0.05527689
H	0.00000000	-2.13890728	-2.02720333
H	0.00000000	2.13890728	-2.02720333

Triplet GeH_2 at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ge	0.00000000	-0.00000000	0.03834941
H	0.00000000	-2.49910092	-1.40641168
H	0.00000000	2.49910092	-1.40641168

Triplet GeH_2 at CCSD(T)/aug-cc-pwCVQZ in bohr			
Ge	0.00000000	-0.00000000	0.03835628
H	0.00000000	-2.49754445	-1.40666345
H	0.00000000	2.49754445	-1.40666345

Singlet AsH_2^+ at CCSD(T)/aug-cc-pwCVTZ in bohr			
As	0.00000000	0.00000000	0.05241727
H	0.00000000	-2.05949199	-1.94834684
H	0.00000000	2.05949199	-1.94834684

Singlet AsH_2^+ at CCSD(T)/aug-cc-pwCVQZ in bohr			
As	0.00000000	0.00000000	0.05238800
H	0.00000000	-2.05872073	-1.94725886
H	0.00000000	2.05872073	-1.94725886

Triplet AsH_2^+ at CCSD(T)/aug-cc-pwCVTZ in bohr			
As	0.00000000	0.00000000	0.03583474
H	0.00000000	-2.48172803	-1.33197534
H	0.00000000	2.48172803	-1.33197534

Triplet AsH_2^+ at CCSD(T)/aug-cc-pwCVQZ in bohr			
As	0.00000000	-0.00000000	0.03583006
H	0.00000000	-2.48042927	-1.33180129
H	0.00000000	2.48042927	-1.33180129

14 Geometry coordinates for the HXCN species

Singlet $HBCN^-$ at CCSD(T)/aug-cc-pVTZ in bohr			
B	-2.81520535	0.23016144	-0.00000000
H	-3.67080706	-1.92138057	-0.00000000
C	0.13253860	-0.05369382	-0.00000000
N	2.36394692	0.00334382	0.00000000

Singlet $HBCN^-$ at CCSD(T)/aug-cc-pVQZ in bohr			
B	-2.80674257	0.22884015	-0.00000000
H	-3.66484891	-1.91783781	-0.00000000
C	0.13203113	-0.05131437	-0.00000000
N	2.35729948	0.00208857	0.00000000

Triplet $HBCN^-$ at CCSD(T)/aug-cc-pVTZ in bohr			
B	-2.71426521	0.17708023	-0.00000000
H	-4.33060919	-1.40123518	-0.00000000
C	0.10663244	-0.01634601	-0.00000000
N	2.35427462	-0.02436453	0.00000000

Triplet $HBCN^-$ at CCSD(T)/aug-cc-pVQZ in bohr			
B	-2.70757058	0.17640524	-0.00000000
H	-4.31894786	-1.40270891	-0.00000000
C	0.10669900	-0.01463044	-0.00000000
N	2.34811494	-0.02519795	0.00000000

Singlet HCCN at aug-cc-pVTZ in bohr			
C	-2.52709950	0.19932664	-0.00000000
H	-3.40498675	-1.68525200	-0.00000000
C	0.09587996	-0.07003074	-0.00000000
N	2.32850768	0.01048973	0.00000000

Singlet HCCN at CCSD(T)/aug-cc-pVQZ in bohr			
C	-2.52050703	0.19780001	-0.00000000
H	-3.40197022	-1.68192953	-0.00000000
C	0.09590280	-0.06706237	-0.00000000
N	2.32262155	0.00901509	0.00000000

Triplet HCCN at CCSD(T)/aug-cc-pVTZ in bohr			
C	-2.43664337	0.12537693	-0.00000000
H	-4.18077463	-0.90399664	-0.00000000
C	0.06917819	-0.04569644	-0.00000000
N	2.32970785	-0.00322040	0.00000000

Triplet HCCN at CCSD(T)/aug-cc-pVQZ in bohr			
C	-2.43005754	0.12362090	-0.00000000
H	-4.17833600	-0.89485418	-0.00000000
C	0.06901281	-0.04391149	-0.00000000
N	2.32403031	-0.00390317	0.00000000

Singlet $HNCN^+$ at CCSD(T)/aug-cc-pVTZ in bohr			
N	-2.25675644	0.16712719	-0.00000000
H	-3.37392877	-1.44250355	-0.00000000
C	0.09957229	-0.09060749	-0.00000000
N	2.41425488	0.01433876	0.00000000

Singlet $HNCN^+$ at CCSD(T)/aug-cc-pVQZ in bohr			
N	-2.25002965	0.16587670	-0.00000000
H	-3.37546092	-1.43396596	-0.00000000
C	0.09883997	-0.08882610	-0.00000000
N	2.40826593	0.01344821	0.00000000

Triplet $HNCN^+$ at CCSD(T)/aug-cc-pVTZ in bohr			
H	-0.00000000	0.00000000	4.11994351
N	-0.00000000	-0.00000000	2.19632940
C	-0.00000000	0.00000000	-0.00896104
N	0.00000000	-0.00000000	-2.48516953

Triplet $HNCN^+$ at CCSD(T)/aug-cc-pVQZ in bohr			
H	-0.00000000	-0.00000000	4.11135305
N	-0.00000000	-0.00000000	2.19020575
C	0.00000000	0.00000000	-0.01008306
N	0.00000000	-0.00000000	-2.47746609

Singlet $HAlCN^-$ at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
Al	-2.47189671	0.13098243	-0.00000000
H	-2.75578889	-3.01685780	-0.00000000
C	1.47727423	-0.08195068	-0.00000000
N	3.69530567	0.03497557	0.00000000

Singlet $HAlCN^-$ at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
Al	-2.46394487	0.13096547	-0.00000000
H	-2.75263767	-3.00923771	-0.00000000
C	1.47251491	-0.08304478	-0.00000000
N	3.68383555	0.03539741	0.00000000

Triplet $HAlCN^-$ at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
Al	-2.36660454	0.12370728	-0.00000000
H	-3.72602847	-2.59670490	-0.00000000
C	1.40378791	-0.02855502	-0.00000000
N	3.62522983	-0.02700323	0.00000000

Triplet $HAlCN^-$ at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
Al	-2.36068009	0.12357935	-0.00000000
H	-3.71562967	-2.59498738	-0.00000000
C	1.40069968	-0.02836101	-0.00000000
N	3.61571247	-0.02704660	0.00000000

Singlet HSiCN at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
Si	-2.23887471	0.11530785	-0.00000000
H	-2.49524440	-2.73288657	-0.00000000
C	1.31550202	-0.07590295	-0.00000000
N	3.52533881	0.03136080	0.00000000

Singlet HSiCN at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
Si	-2.23216182	0.11558903	-0.00000000
H	-2.49401070	-2.72788141	-0.00000000
C	1.31178422	-0.07811208	-0.00000000
N	3.51502422	0.03233193	0.00000000

Triplet HSiCN at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
Si	-2.16656759	0.11074317	-0.00000000
H	-3.51953907	-2.33415869	-0.00000000
C	1.27510250	-0.03897314	-0.00000000
N	3.48921623	-0.01986366	0.00000000

Triplet HSiCN at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
Si	-2.16089579	0.11070128	-0.00000000
H	-3.50507132	-2.33508193	-0.00000000
C	1.27183308	-0.03894145	-0.00000000
N	3.47964494	-0.01974068	0.00000000

Singlet $HPCN^+$ at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
P	-1.99186027	0.10088481	-0.00000000
H	-2.31851292	-2.57176176	-0.00000000
C	1.26088852	-0.07752515	-0.00000000
N	3.49219030	0.02837987	0.00000000

Singlet $HPCN^+$ at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
P	-1.98645088	0.10108940	-0.00000000
H	-2.31747588	-2.56897889	-0.00000000
C	1.25803812	-0.07894381	-0.00000000
N	3.48259315	0.02894278	0.00000000

Triplet $HPCN^+$ at CCSD(T)/aug-cc-pV(T+d)Z in bohr			
P	-1.95075065	0.10127812	-0.00000000
H	-3.33686595	-2.19417325	-0.00000000
C	1.24886387	-0.07327617	-0.00000000
N	3.48485604	-0.00330696	0.00000000

Triplet $HPCN^+$ at CCSD(T)/aug-cc-pV(Q+d)Z in bohr			
P	-1.94561342	0.10116140	-0.00000000
H	-3.32464619	-2.19616048	-0.00000000
C	1.24577240	-0.07232406	-0.00000000
N	3.47526265	-0.00372167	0.00000000

Singlet $HGaCN^-$ at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ga	-1.41793356	0.05451793	-0.00000000
H	-1.63203901	-3.10707840	-0.00000000
C	2.63065445	-0.12246388	-0.00000000
N	4.84242599	0.06022090	0.00000000

Singlet $HGaCN^-$ at CCSD(T)/aug-cc-pwCVQZ in bohr			
Ga	-1.41366848	0.05479752	-0.00000000
H	-1.63631794	-3.10222787	-0.00000000
C	2.62212346	-0.12704130	-0.00000000
N	4.82905116	0.06241825	0.00000000

Triplet $HGaCN^-$ at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ga	-1.32830029	0.05073724	-0.00000000
H	-2.72864493	-2.58376083	-0.00000000
C	2.43217844	-0.06360872	-0.00000000
N	4.65024490	-0.00927013	0.00000000

Triplet $HGaCN^-$ at CCSD(T)/aug-cc-pwCVQZ in bohr			
Ga	-1.32567877	0.05089646	-0.00000000
H	-2.72950826	-2.58061806	-0.00000000
C	2.42746187	-0.06634414	-0.00000000
N	4.64144533	-0.00793591	0.00000000

Singlet HGeCN at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ge	-1.26253784	0.04670079	-0.00000000
H	-1.44177054	-2.92603349	-0.00000000
C	2.45786135	-0.09273326	-0.00000000
N	4.66233342	0.04352981	0.00000000

Singlet HGeCN at CCSD(T)/aug-cc-pwCVQZ in bohr			
Ge	-1.26014180	0.04690622	-0.00000000
H	-1.44336300	-2.92374155	-0.00000000
C	2.45352219	-0.09619776	-0.00000000
N	4.65351796	0.04524933	0.00000000

Triplet HGeCN at CCSD(T)/aug-cc-pwCVTZ in bohr			
Ge	-1.21303305	0.04587932	-0.00000000
H	-2.59853761	-2.48188256	-0.00000000
C	2.35958971	-0.06341208	-0.00000000
N	4.56847020	-0.00922689	0.00000000

Triplet HGeCN at CCSD(T)/aug-cc-pwCVQZ in bohr			
Ge	-1.21093422	0.04596381	-0.00000000
H	-2.59623291	-2.48033657	-0.00000000
C	2.35573079	-0.06499517	-0.00000000
N	4.56053165	-0.00842757	0.00000000

Singlet $HAsCN^+$ at CCSD(T)/aug-cc-pwCVTZ in bohr			
As	-1.19199192	0.04471743	-0.00000000
H	-1.42383092	-2.82391453	-0.00000000
C	2.29378222	-0.08322960	-0.00000000
N	4.51440309	0.03531125	0.00000000

Singlet $HAsCN^+$ at CCSD(T)/aug-cc-pwCVQZ in bohr			
As	-1.18976032	0.04497071	-0.00000000
H	-1.42710792	-2.82199166	-0.00000000
C	2.28990413	-0.08710460	-0.00000000
N	4.50602240	0.03713842	0.00000000

Triplet $HAsCN^+$ at CCSD(T)/aug-cc-pwCVTZ in bohr			
As	-1.16638298	0.04579275	-0.00000000
H	-2.55950750	-2.45097238	-0.00000000
C	2.26197373	-0.07453156	-0.00000000
N	4.48638085	-0.00473721	0.00000000

Triplet $HAsCN^+$ at CCSD(T)/aug-cc-pwCVQZ in bohr			
As	-1.16408698	0.04590494	-0.00000000
H	-2.55957148	-2.44791213	-0.00000000
C	2.25763168	-0.07665767	-0.00000000
N	4.47782196	-0.00373578	0.00000000

15 Singlet NBO values for HXCN

$HBCN^-$	E2	E(j) – E(i)	F(i,j)
(3) C-N -> LP*(2) X	11.11	0.34	0.055
LP(1)X -> (1)* C-N	7.02	1.08	0.082
LP(1)X -> (2)* C-N	22.17	0.28	0.071
LP(1) N -> (1)*X-C	10.78	0.92	0.089
	% s/ % p/% d		
LP(1) X	53.06/46.73/0		
LP*(2) X	0/99.25/0.75		
LP(1)N	50.72/49.13/0		

HCCN	E2	E(j) – E(i)	F(i,j)
(3) C-N -> LP*(2) X	43.80	0.24	0.092
LP(1)X -> (1)* C-N	11.78	1.17	0.109
LP(1)X -> (2)* C-N	14.88	0.44	0.072
LP(1) N -> (1)*X-C	12.96	1.09	0.106
	% s/ % p/% d		
LP(1) X	50.58/49.13/0		
LP*(2) X	0/99.38/0.62		
LP(1)N	56.52/43.33/0		

$HNCN^+$	E2	E(j) – E(i)	F(i,j)
(2) N1-C -> LP*(2) N4	101.26	0.20	0.128
LP(1)N1 -> (1)* C-N4	12.38	1.11	0.108
LP(1)N1 -> (2)* C-N4	13.15	0.58	0.078
LP(1) N4 -> (1)*N1-C	15.81	1.23	0.125
	% s/ % p/% d		
LP(1) X	44.15/55.54/0		
LP(1) N	67.66/32.23/0		
LP*(2)N	0/99.34/0.66/0		

$HAlCN^-$	E2	E(j) – E(i)	F(i,j)
(3) C-N -> LP*(2)	2.14	0.32	0.023
LP(1)X -> (1)* C-N	4.56	1.14	0.065
LP(1)X -> (2)* C-N	5.84	0.38	0.042
LP(1) N -> (1)*X-C	5.93	0.65	0.056
	% s/ % p/% d		
LP(1) X	77.33/22.5/0		
LP*(2) X	0/96.61/3.39		
LP(1)N	49.19/50.63/0		

HSiCN	E2	E(j) – E(i)	F(i,j)
(3) C-N -> LP*(2)	9.44	0.26	0.045
LP(1)X -> (1)* C-N	9.00	1.32	0.098
LP(1)X -> (2)* C-N	3.88	0.51	0.040
LP(1) N -> (1)*X-C	7.51	0.73	0.066
	% s/ % p/% d		
LP(1) X	78.48/21.40/0		
LP*(2) X	0/96.46/3.54		
LP(1)N	52.05/47.77/0		

$HPCN^+$	E2	E(j) – E(i)	F(i,j)
(3) C-N -> LP*(2)	39.98	0.17	0.074
LP(1)X -> (1)* C-N	11.87	1.44	0.117
LP(1)X -> (2)* C-N	2.93	0.66	0.040
LP(1) N -> (1)*X-C	10.50	0.80	0.082
	% s/ % p/% d		
LP(1) X	75.79/24.07/0		
LP*(2) X	0/97.56/2.44		
LP(1)N	57.71/42.11/0		

$HGaCN^-$	E2	E(j) – E(i)	F(i,j)
(3) C-N -> LP*(2)	1.89	0.29	0.021
LP(1)X -> (1)* C-N	5.64	1.26	0.076
LP(1)X -> (2)* C-N	5.33	0.45	0.044
LP(1) N -> (1)*X-C	5.92	0.62	0.054
	% s/ % p/% d		
LP(1) X	81.79/18.11/0		
LP*(2) X	0/98.74/1.23		
LP(1)N	49.31/50.50/0		

HGeCN	E2	E(j) – E(i)	F(i,j)
(3) C-N -> LP*(2)	7.47	0.24	0.038
LP(1)X -> (1)* C-N	10.11	1.45	0.108
LP(1)X -> (2)* C-N	2.78	0.60	0.037
LP(1) N -> (1)*X-C	6.99	0.67	0.061
	% s/ % p/% d		
LP(1) X	82.89/17.06/0		
LP*(2) X	0/98.58/1.41		
LP(1)N	51.96/47.84/0		

$HAsCN^+$	E2	E(j) – E(i)	F(i,j)
(3) C-N -> LP*(2)	28.46	0.16	0.060
LP(1)X -> (1)* C-N	12.74	1.57	0.127
LP(1)X -> (2)* C-N	1.73	0.77	0.033
LP(1) N -> (1)*X-C	9.51	0.70	0.073
	% s/ % p/% d		
LP(1) X	81.43/18.50/0		
LP*(2) X	0/98.64/1.36		
LP(1)N	56.86/42.95/0		

Figure 1: E(2) is in kcal mol^{-1}. E(j) - E(i) and F(i,j) are in hartrees.

16 Triplet NBO values for HXCN

$HBCN^-$	E2	E(j) – E(i)	F(i,j)
LP(1)X -> (1)* C-N	2.59	1.06	0.070
LP(1)X -> (3)* C-N	19.86	0.29	0.096
LP(2)X -> (2)* C-N	48.87	0.19	0.121
LP(1) N -> (1)*X-C	5.87	0.99	0.097
(2) C-N -> LP*(2) X	6.53	0.35	0.060
(3) C-N -> LP*(1) X	7.45	0.36	0.065
LP(1) N -> (1)*X-C	5.68	0.99	0.095
% s/ % p/% d			
LP(1) X 33.38/66.53/0			
LP(2) X 0/99.91/0.09			
LP(1)N 51.81/48.03/0			
LP*(1) X 0/99.38/0.62			
LP*(2) X 7.64/91.67/0.69			
LP(1)N 50.72/49.16/0			

HCCN	E2	E(j) – E(i)	F(i,j)
LP(1)X -> (1)* C-N	3.71	1.10	0.086
LP(1)X -> (3)* C-N	22.76	0.39	0.119
LP(2)X -> (2)* C-N	54.34	0.28	0.156
LP(1) N -> (1)*X-C	7.26	1.24	0.120
(2) C-N -> LP*(2) X	28.41	0.26	0.109
(3) C-N -> LP*(1) X	28.87	0.27	0.112
LP(1) N -> (1)*X-C	6.74	1.22	0.115
% s/ % p/% d			
LP(1) X 22.25/77.70/0			
LP(2) X 0/99.93/0.07			
LP(1)N 58.91/40.92/0			
LP*(1) X 0/99.67/0.33			
LP*(2) X 3.09/96.57/0.34			
LP(1)N 57.23/42.66/0			

$HNCN^+$	E2	E(j) – E(i)	F(i,j)
LP(1)N -> (1)* X-C	9.02	1.56	0.150
LP(2)N -> (3)* X-C	49.92	0.31	0.158
LP(3)N -> (2)* X-C	949.92	0.31	0.158
(2) X-C -> LP*(2) N	17.74	0.32	0.095
(3) X-C -> LP*(3) N	17.74	0.32	0.095
LP(1) N -> (1)*X-C	8.21	1.46	0.139
% s/ % p/% d			
LP(1) N 77.20/22.68/0			
LP(2) N 0/99.43/0.57			
LP(3) N 0/9943/0.57			
LP(1) N 73.90/26.07/0			
LP*(2) N 0/99.46/0.54			
LP*(3) N 0/99.46/0.54			

$HAlCN^-$	E2	E(j) – E(i)	F(i,j)
LP(1)X -> (1)* C-N	3.39	1.15	0.079
LP(1)X -> (3)* C-N	3.08	0.35	0.042
LP(2)X -> (2)* C-N	12.61	0.21	0.065
LP(1) N -> (1)*X-C	3.27	0.66	0.059
(2) C-N -> LP*(2) X	1.40	0.39	0.029
(3) C-N -> LP*(1) X	1.45	0.36	0.029
LP(1) N -> (1)*X-C	3.76	0.65	0.063
% s/ % p/% d			
LP(1) X 65.33/34.42/0			
LP(2) X 0/99.77/0.23			
LP(1)N 49.13/50.69/0			
LP*(1) X 0/96.95/3.05			
LP*(2) X 6.44/90.56/3.01			
LP(1)N 49.20/50.64/0			

HSiCN	E2	E(j) – E(i)	F(i,j)
LP(1)X -> (1)* C-N	4.93	1.28	0.101
LP(1)X -> (3)* C-N	2.20	0.47	0.041
LP(2)X -> (2)* C-N	18.85	0.26	0.088
LP(1) N -> (1)*X-C	4.05	0.76	0.070
(2) C-N -> LP*(2) X	4.88	0.32	0.049
(3) C-N -> LP*(1) X	5.10	0.33	0.052
LP(1) N -> (1)*X-C	4.92	0.74	0.076
% s/ % p/% d			
LP(1) X 65.92/33.96/0			
LP(2) X 0/99.97/0.03			
LP(1)N 52.17/47.64/0			
LP*(1) X 4.77/91.82/3.41			
LP*(2) X 0/96.04/3.96			
LP(1)N 52.29/47.54/0			

$HPCN^+$	E2	E(j) – E(i)	F(i,j)
LP(1)X -> (1)* C-N	5.78	1.36	0.113
LP(1)X -> (3)* C-N	2.03	0.60	0.044
LP(2)X -> (2)* C-N	20.12	0.32	0.102
LP(1) N -> (1)*X-C	5.53	0.83	0.086
(2) C-N -> LP*(2) X	16.08	0.23	0.077
(3) C-N -> LP*(1) X	23.95	0.21	0.090
LP(1) N -> (1)*X-C	7.14	0.79	0.095
% s/ % p/% d			
LP(1) X 65.35/34.54/0.11			
LP(2) X 0/99.96/0.04			
LP(1)N 58.47/41.34/0.19			
LP*(1) X 3.49/94.68/1.83			
LP*(2) X 0/96.77/3.23			
LP(1)N 58.19/41.67/0.14			

$HGaCN^-$	E2	E(j) – E(i)	F(i,j)
LP(1)X -> (1)* C-N	4.20	1.22	0.091
LP(1)X -> (2)* C-N	3.44	0.39	0.046
LP(2)X -> (3)* C-N	13.03	0.21	0.065
LP(1) N -> (1)*X-C	3.48	0.65	0.060
(2) C-N -> LP*(1) X	1.55	0.39	0.031
(3) C-N -> LP*(2) X	1.50	0.34	0.028
LP(1) N -> (1)*X-C	4.24	0.64	0.066
% s/ % p/% d/% f			
LP(1) X 68.14/31.73/0/0			
LP(2) X 0/99.89/0.11/0/0			
LP(1)N 49.28/50.53/0/0			
LP*(1) X 4.64/94.6/0.71/0.05			
LP*(2) X 0/99.19/0.76/0.05			
LP(1)N 49.49/50.34/0.17/0			

HGeCN	E2	E(j) – E(i)	F(i,j)
LP(1)X -> (1)* C-N	5.90	1.35	0.113
LP(1)X -> (3)* C-N	1.37	0.52	0.034
LP(2)X -> (2)* C-N	16.26	0.26	0.082
LP(1) N -> (1)*X-C	3.81	0.70	0.065
(2) C-N -> LP*(2) X	3.93	0.29	0.043
(3) C-N -> LP*(1) X	4.42	0.32	0.048
LP(1) N -> (1)*X-C	5.12	0.68	0.075
% s/ % p/% d/% f			
LP(1) X 71.48/28.48/0.04/0			
LP(2) X 0/99.97/0.03/0/0			
LP(1)N 52.08/47.72/0.2/0			
LP*(1) X 3.47/95.44/1.06/0.02			
LP*(2) X 0/98.61/1.37/0.03			
LP(1)N 52.55/47.28/0.17/0			

$HAsCN^+$	E2	E(j) – E(i)	F(i,j)
LP(1)X -> (1)* C-N	6.66	1.44	0.124
LP(1)X -> (3)* C-N	0.88	0.67	0.031
LP(2)X -> (2)* C-N	15.60	0.32	0.089
LP(1) N -> (1)*X-C	4.87	0.73	0.076
(1) C-N -> LP*(1) X	0.27	0.89	0.021
(2) C-N -> LP*(2) X	10.21	0.23	0.061
(3) C-N -> LP*(1) X	17.19	0.22	0.078
LP(1) N -> (1)*X-C	7.57	0.69	0.092
% s/ % p/% d/% f			
LP(1) X 73.33/26.63/0.04/0			
LP(2) X 0/99.97/0.03/0			
LP(1)N 57.39/42.41/0.2/0			
LP*(1) X 2.50/96.69/0.80/0.01			
LP*(2) X 0/98.24/1.75/0.01			
LP(1)N 57.93/41.92/0.15/0			

Figure 2: E(2) is in kcal mol^{-1}. E(j) - E(i) and F(i,j) are in hartrees. Black values are for alpha electrons, red values are for beta electrons.