

Supplementary material

Fig. S1 illustrates the most energetically favorable adsorption sites of NO₂, CO, NH₃, PH₃, HCN, and H₂O onto the pristine G/h-BN/G nanopore, along with their respective distances from the surface.

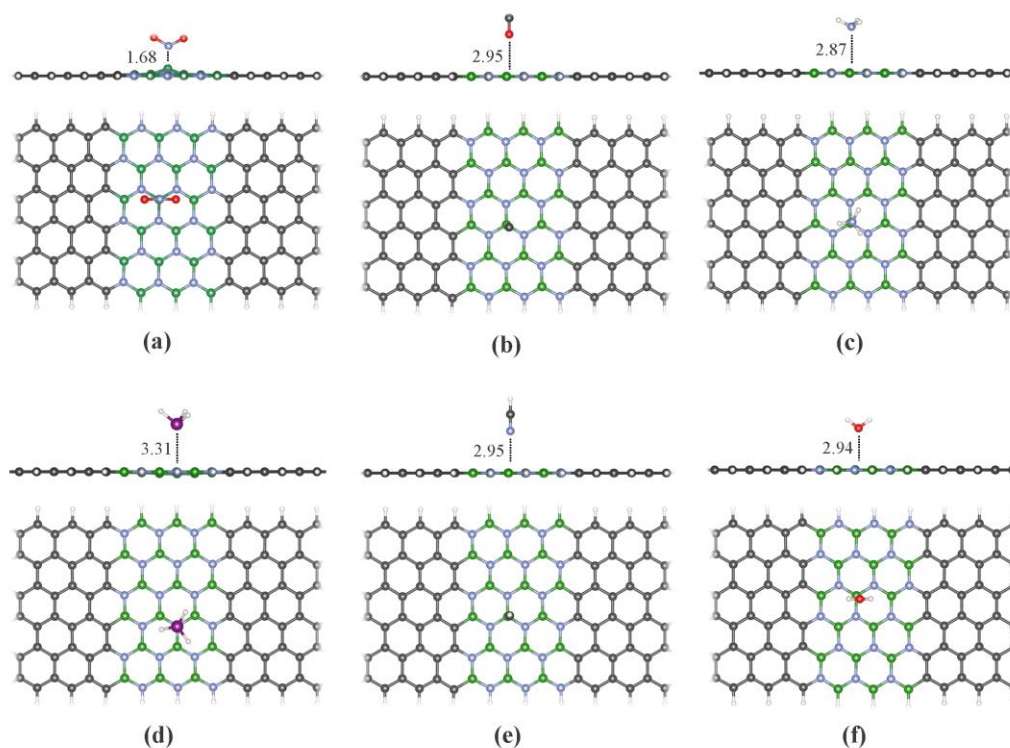


Figure S1: The most energetically favored geometries for the adsorption of gas molecules onto the Pristine G/h-BN/G structure. Distances are presented in angstroms, and the gas molecules include (a) NO₂, (b) CO, (c) NH₃, (d) PH₃, (e) HCN, and (f) H₂O.

The electron transmission spectrum of doped structures in the presence of NH₃, PH₃, and HCN molecules is depicted in Fig. S2.

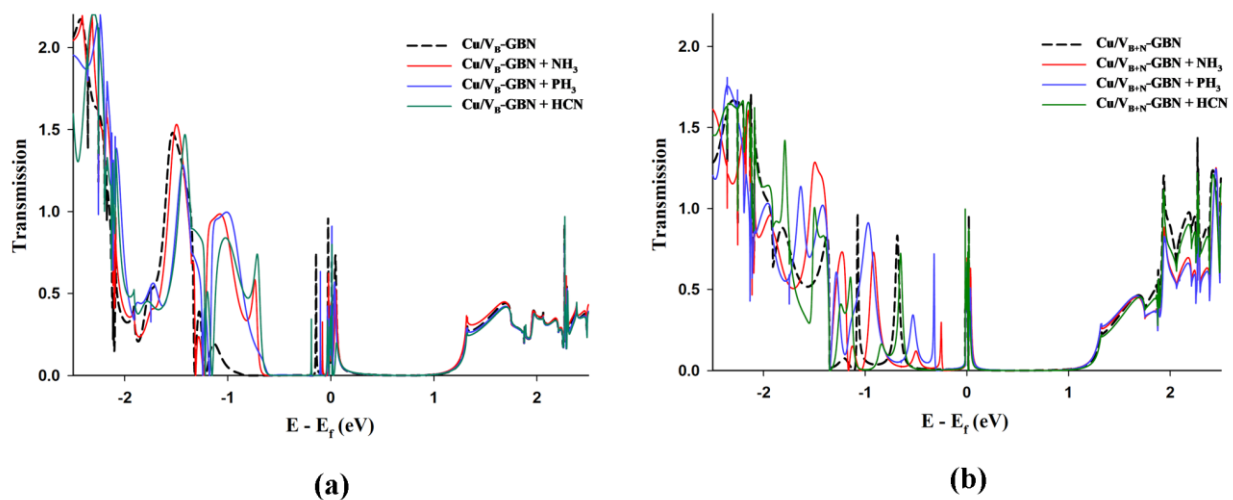


Figure S2: Transmission spectrum of Cu-doped structures, with and without NH_3 , PH_3 , and HCN molecules at zero bias voltage. (a) $\text{Cu/V}_\text{B}\text{-GBN}$, (b) $\text{Cu/V}_{\text{B+N}}\text{-GBN}$

Cartesian Coordinates

The Cartesian coordinates of the optimized geometries $\text{Cu/V}_\text{B}\text{-GBN}$ and $\text{Cu/V}_{\text{B+N}}\text{-GBN}$, both with and without gas molecules, are presented. The coordinates are provided for the most energetically favorable adsorption sites of NO_2 , CO , NH_3 , PH_3 , and HCN molecules.

Cu/V_B-GBN

C	49.200000	2.010100	1.230000	C	49.668428	1.388533	12.279700	C	49.218161	6.345869	23.374793
C	49.200000	3.468530	1.230000	C	49.140615	4.239842	12.267958	C	49.273867	7.780817	23.365118
C	49.200000	6.360240	1.230000	C	48.922037	5.661142	12.313301	C	49.507140	10.651645	23.386310
C	49.200000	7.804660	1.230000	C	49.001925	8.561294	12.276491	C	49.657454	12.094283	23.375250
C	49.200000	10.697170	1.229980	C	49.119419	9.996030	12.288473	H	49.697586	13.896976	24.602019
C	49.200000	12.144060	1.229990	C	49.544853	12.880166	12.243277	H	49.284420	0.222841	24.605233
H	49.200000	13.991190	2.460000	N	49.535117	1.996577	13.489994	C	49.267395	1.327870	24.609649
H	49.200000	0.204130	2.460000	B	49.215774	3.433145	13.538718	C	49.226864	4.191272	24.603910
C	49.200000	1.312260	2.460000	N	48.586433	6.287418	13.518547	C	49.231021	5.633074	24.606275
C	49.200000	4.189910	2.460000	B	48.580435	7.784297	13.539811	C	49.312165	8.503545	24.601760
C	49.200000	5.636640	2.460000	N	49.037361	10.697320	13.488708	C	49.392410	9.943366	24.612567
C	49.200000	8.528800	2.460000	B	49.272894	12.141388	13.528570	C	49.611879	12.795220	24.600031
C	49.200000	9.973320	2.459980	H	49.436247	13.803808	14.793620	C	49.233239	2.021825	25.837390
C	49.200000	12.865540	2.460000	H	49.933175	0.049210	14.676875	C	49.228282	3.475536	25.830498
C	49.200000	2.010100	3.690000	B	49.648309	1.238005	14.722689	C	49.236633	6.352926	25.834696
C	49.200000	3.468530	3.690000	N	48.951316	4.073028	14.764086	C	49.259508	7.794572	25.832153
C	49.200000	6.360240	3.690000	B	48.416738	5.444483	14.762954	C	49.352706	10.667639	25.835199
C	49.200000	7.804660	3.690000	N	48.157766	8.646045	14.578829	C	49.424730	12.118128	25.827603
C	49.200000	10.697170	3.689980	B	48.610442	9.989073	14.708355	H	49.350838	13.926645	27.045489
C	49.200000	12.144060	3.690000	N	49.219461	12.808742	14.784753	H	49.212090	0.214858	27.049886
H	49.200000	13.991190	4.920000	N	49.416824	1.921871	15.951765	C	49.213441	1.320630	27.059862
H	49.200000	0.204130	4.920000	B	49.045717	3.345463	15.992610	C	49.214529	4.191099	27.065190
C	49.200000	1.312260	4.920000	N	47.822545	5.899421	15.950840	C	49.216218	5.634439	27.064616
C	49.200000	4.189910	4.920000	Cu	47.276388	7.748148	16.001616	C	49.233365	8.522502	27.063118
C	49.200000	5.636640	4.920000	N	48.701634	10.697316	15.979188	C	49.250873	9.965853	27.066820
C	49.200000	8.528800	4.920000	B	49.062724	12.106698	16.013299	C	49.314496	12.821684	27.051512
C	49.200000	9.973320	4.919980	H	49.523646	13.776660	17.233643	C	49.200000	2.010100	28.290000
C	49.200000	12.865540	4.920000	H	49.803636	-0.000239	17.180922	C	49.200000	3.468530	28.290000
C	49.266047	2.014336	6.149697	B	49.538057	1.193008	17.184616	C	49.200000	6.360240	28.290000
C	49.238987	3.475308	6.150348	N	48.829330	4.027140	17.235227	C	49.200000	7.804660	28.290000
C	49.209903	6.365798	6.145884	B	48.344324	5.427909	17.178913	C	49.200000	10.697170	28.289980
C	49.211142	7.807852	6.145450	N	48.220298	8.619593	17.401968	C	49.200000	12.144060	28.290000
C	49.247681	10.697349	6.141788	B	48.651995	9.964447	17.243321	H	49.200000	13.991190	29.520000
C	49.273618	12.156596	6.138322	N	49.292104	12.785589	17.255819	H	49.200000	0.204130	29.520000
H	49.454670	13.943782	7.368538	N	49.353256	1.897045	18.423469	C	49.200000	1.312260	29.520000
H	49.462077	0.239600	7.408121	B	49.057885	3.328347	18.451409	C	49.200000	4.189910	29.520000
C	49.390203	1.342454	7.389040	N	48.510075	6.245375	18.405987	C	49.200000	5.636640	29.520000
C	49.259498	4.207936	7.373611	B	48.551095	7.731456	18.457300	C	49.200000	8.528800	29.520000
C	49.226317	5.653000	7.382510	N	49.105798	10.640292	18.445909	C	49.200000	9.973320	29.519980
C	49.233365	8.533631	7.371365	B	49.375921	12.058502	18.474231	C	49.200000	12.865540	29.520000
C	49.276756	9.976359	7.373174	H	49.857791	13.717006	19.745724	C	49.200000	2.010100	30.750000
C	49.401408	12.839779	7.364587	H	49.645364	-0.024403	19.663243	C	49.200000	3.468530	30.750000
C	49.437144	2.052065	8.610041	B	49.440039	1.183727	19.655020	C	49.200000	6.360240	30.750000
C	49.326474	3.505914	8.606883	N	48.991629	4.087956	19.692367	C	49.200000	7.804660	30.750000
C	49.211835	6.380251	8.609909	B	48.839257	5.556028	19.625869	C	49.200000	10.697170	30.749980
C	49.217527	7.821425	8.602053	N	48.980633	8.434919	19.698731	C	49.200000	12.144060	30.749990
C	49.353810	10.687883	8.599844	B	49.191692	9.881236	19.655697	H	49.200000	13.991190	31.980000
C	49.456743	12.138447	8.585839	N	49.706639	12.710183	19.709688	H	49.200000	0.204130	31.980000
H	49.704112	13.927847	9.795666	C	49.290580	2.000709	20.939664	C	49.200000	1.312260	31.980000
H	49.730520	0.286093	9.855554	C	49.144979	3.439360	20.912881	C	49.200000	4.189910	31.980000
C	49.591880	1.382993	9.844475	C	49.033229	6.344182	20.922106	C	49.200000	5.636640	31.980000
C	49.281173	4.234933	9.824716	C	49.100059	7.770875	20.911911	C	49.200000	8.528800	31.979990
C	49.190046	5.671133	9.853332	C	49.477929	10.643741	20.937311	C	49.200000	9.973320	31.979980
C	49.215470	8.545362	9.827740	C	49.677864	12.067754	20.935752	C	49.200000	12.865540	31.980000
C	49.309856	9.980092	9.838028	H	49.927320	13.872913	22.129131				
C	49.588254	12.828481	9.801664	H	49.437937	0.229372	22.161101				
C	49.541901	2.092398	11.067860	C	49.340139	1.331189	22.157557				
C	49.326983	3.539994	11.062994	C	49.162392	4.182249	22.131382				
C	49.064253	6.393819	11.085613	C	49.140168	5.633845	22.137399				
C	49.094286	7.843721	11.065562	C	49.275914	8.498421	22.132835				
C	49.323738	10.705012	11.069181	C	49.432335	9.939228	22.154399				
C	49.505576	12.157701	11.047562	C	49.793682	12.775526	22.133846				
H	49.711076	13.972537	12.181434	C	49.272099	2.026257	23.391339				
H	49.864259	0.299321	12.281934	C	49.223508	3.472839	23.367576				

Cu/V_B-GBN + NO₂

C	49.200000	2.010100	1.230000	C	49.793680	12.775530	22.133850	B	48.881282	5.563052	19.625454
C	49.200000	3.468530	1.230000	C	49.657450	12.094280	23.375250	N	49.020093	8.440506	19.689624
C	49.200000	6.360240	1.230000	H	49.697590	13.896980	24.602020	B	49.214537	9.883786	19.656972
C	49.200000	7.804660	1.230000	H	49.284420	0.222840	24.605230	N	44.686287	7.559192	16.045304
C	49.200000	10.697170	1.229980	C	49.267400	1.327870	24.609650	O	45.534392	7.439759	17.027552
C	49.200000	12.144060	1.229990	C	49.611880	12.795220	24.600030	O	45.303300	7.933251	14.979820
H	49.200000	13.991190	2.460000	C	49.424730	12.118130	25.827600	C	49.293321	2.002797	20.939296
H	49.200000	0.204130	2.460000	H	49.350840	13.926650	27.045490	C	49.152068	3.442144	20.910489
C	49.200000	1.312260	2.460000	H	49.212090	0.214860	27.049890	C	49.060732	6.349602	20.921361
C	49.200000	4.189910	2.460000	C	49.213440	1.320630	27.059860	C	49.127689	7.774875	20.903702
C	49.200000	5.636640	2.460000	C	49.314500	12.821680	27.051510	C	49.487117	10.646651	20.941199
C	49.200000	8.528800	2.460000	C	49.264328	2.016660	6.151467	C	49.159450	4.185549	22.131216
C	49.200000	9.973320	2.459980	C	49.235813	3.475076	6.148770	C	49.145509	5.637584	22.137666
C	49.200000	12.865540	2.460000	C	49.209730	6.366392	6.146101	C	49.288981	8.501267	22.131166
C	49.200000	2.010100	3.690000	C	49.213428	7.807373	6.147101	C	49.440376	9.940893	22.156720
C	49.200000	3.468530	3.690000	C	49.248896	10.699152	6.143330	C	49.266263	2.027778	23.388967
C	49.200000	6.360240	3.690000	C	49.254764	4.207757	7.371714	C	49.209169	3.473495	23.366116
C	49.200000	7.804660	3.690000	C	49.224964	5.652325	7.379962	C	49.211190	6.348692	23.374918
C	49.200000	10.697170	3.689980	C	49.241382	8.533328	7.372143	C	49.275378	7.782992	23.362475
C	49.200000	12.144060	3.690000	C	49.282204	9.976219	7.374089	C	49.509502	10.653836	23.387787
H	49.200000	13.991190	4.920000	C	49.434762	2.052006	8.611604	C	49.202277	4.192495	24.603491
H	49.200000	0.204130	4.920000	C	49.320726	3.504473	8.603404	C	49.208367	5.634163	24.605789
C	49.200000	1.312260	4.920000	C	49.216001	6.380904	8.606033	C	49.308457	8.505990	24.601590
C	49.200000	4.189910	4.920000	C	49.228497	7.820478	8.603352	C	49.393100	9.944432	24.613137
C	49.200000	5.636640	4.920000	C	49.357811	10.689716	8.601053	C	49.224790	2.022543	25.834989
C	49.200000	8.528800	4.920000	C	49.279881	4.233480	9.820746	C	49.206972	3.475563	25.829723
C	49.200000	9.973320	4.919980	C	49.197571	5.669945	9.846751	C	49.216126	6.353957	25.835062
C	49.200000	12.865540	4.920000	C	49.227249	8.544886	9.832313	C	49.248975	7.795317	25.831738
C	49.273620	12.156600	6.138320	C	49.314853	9.979750	9.843092	C	49.352653	10.668977	25.835903
H	49.454670	13.943780	7.368540	C	49.542288	2.088666	11.068754	C	49.199001	4.192030	27.063959
H	49.462080	0.239600	7.408120	C	49.333329	3.534568	11.056631	C	49.200838	5.634406	27.063253
C	49.390200	1.342450	7.389040	C	49.096906	6.393314	11.075957	C	49.229884	8.523418	27.062328
C	49.401410	12.839780	7.364590	C	49.119345	7.841449	11.069288	C	49.250870	9.965850	27.066820
C	49.456740	12.138450	8.585840	C	49.327178	10.705290	11.072408	C	49.200000	2.010100	28.290000
H	49.704110	13.927850	9.795670	C	49.175721	4.235125	12.261140	C	49.200000	3.468530	28.290000
H	49.730520	0.286090	9.855550	C	48.987223	5.656521	12.299664	C	49.200000	6.360240	28.290000
C	49.591880	1.382990	9.844470	C	49.033098	8.561435	12.285168	C	49.200000	7.804660	28.290000
C	49.588250	12.828480	9.801660	C	49.135469	9.991059	12.297317	C	49.200000	10.697170	28.289980
C	49.505580	12.157700	11.047560	N	49.538554	1.996312	13.493463	C	49.200000	12.144060	28.290000
H	49.711080	13.972540	12.181430	B	49.249444	3.432249	13.536704	H	49.200000	13.991190	29.520000
H	49.864260	0.299320	12.281930	N	48.715792	6.285856	13.504749	H	49.200000	0.204130	29.520000
C	49.668430	1.388530	12.279700	B	48.698766	7.755785	13.561493	C	49.200000	1.312260	29.520000
C	49.544850	12.880170	12.243280	N	49.050827	10.687978	13.500180	C	49.200000	4.189910	29.520000
B	49.272890	12.141390	13.528570	N	49.025788	4.083895	14.762153	C	49.200000	5.636640	29.520000
H	49.436250	13.803810	14.793620	B	48.578964	5.481111	14.760636	C	49.200000	8.528800	29.520000
H	49.933170	0.049210	14.676880	N	48.378696	8.577725	14.666924	C	49.200000	9.973320	29.519980
B	49.648310	1.238010	14.722690	B	48.694741	9.969066	14.741676	C	49.200000	12.865540	29.520000
N	49.219460	12.808740	14.784750	N	49.428490	1.925573	15.954004	C	49.200000	2.010100	30.750000
B	49.062720	12.106700	16.013300	B	49.096706	3.359265	15.992193	C	49.200000	3.468530	30.750000
H	49.523650	13.776660	17.233640	N	48.091341	6.040029	15.930300	C	49.200000	6.360240	30.750000
H	49.803640	-0.000240	17.180920	Cu	47.170418	7.875272	15.950445	C	49.200000	7.804660	30.750000
B	49.538060	1.193010	17.184620	N	48.725882	10.701995	15.986672	C	49.200000	10.697170	30.749980
N	49.292100	12.785590	17.255820	N	48.889708	4.054714	17.228303	C	49.200000	12.144060	30.749990
B	49.375920	12.058500	18.474230	B	48.480085	5.485636	17.161844	H	49.200000	13.991190	31.980000
H	49.857790	13.717010	19.745720	N	48.313528	8.610972	17.363091	H	49.200000	0.204130	31.980000
H	49.645360	-0.024400	19.663240	B	48.695615	9.961457	17.243310	C	49.200000	1.312260	31.980000
B	49.440040	1.183730	19.655020	N	49.353603	1.901212	18.423445	C	49.200000	4.189910	31.980000
N	49.706640	12.710180	19.709690	B	49.081445	3.339722	18.444552	C	49.200000	5.636640	31.980000
C	49.677860	12.067750	20.935750	N	48.588938	6.262333	18.408809	C	49.200000	8.528800	31.979990
H	49.927320	13.872910	22.129130	B	48.617300	7.733917	18.436810	C	49.200000	9.973320	31.979980
H	49.437940	0.229370	22.161100	N	49.122603	10.641598	18.450980	C	49.200783	12.859204	31.980371
C	49.340140	1.331190	22.157560	N	49.016947	4.094516	19.690225				

Cu/V_B-GBN + NH₃

C	49.200000	2.010100	1.230000	C	49.793680	12.775530	22.133850	B	48.865623	5.562328	19.628152
C	49.200000	3.468530	1.230000	C	49.657450	12.094280	23.375250	N	49.035772	8.439517	19.695901
C	49.200000	6.360240	1.230000	H	49.697590	13.896980	24.602020	B	49.225043	9.885014	19.657144
C	49.200000	7.804660	1.230000	H	49.284420	0.222840	24.605230	N	45.513585	7.478716	17.230863
C	49.200000	10.697170	1.229980	C	49.267400	1.327870	24.609650	H	45.900953	6.894308	17.985689
C	49.200000	12.144060	1.229990	C	49.611880	12.795220	24.600030	H	44.693402	6.993250	16.850172
H	49.200000	13.991190	2.460000	C	49.424730	12.118130	25.827600	H	45.204268	8.358783	17.659154
H	49.200000	0.204130	2.460000	H	49.350840	13.926650	27.045490	C	49.295704	2.001856	20.939463
C	49.200000	1.312260	2.460000	H	49.212090	0.214860	27.049890	C	49.159775	3.441875	20.911948
C	49.200000	4.189910	2.460000	C	49.213440	1.320630	27.059860	C	49.078052	6.347484	20.920794
C	49.200000	5.636640	2.460000	C	49.314500	12.821680	27.051510	C	49.150602	7.774299	20.908647
C	49.200000	8.528800	2.460000	C	49.266731	2.014487	6.150060	C	49.493400	10.644964	20.940387
C	49.200000	9.973320	2.459980	C	49.242910	3.475224	6.150282	C	49.183651	4.184576	22.130164
C	49.200000	12.865540	2.460000	C	49.219007	6.365558	6.146404	C	49.173871	5.636919	22.135922
C	49.200000	2.010100	3.690000	C	49.220464	7.807748	6.145846	C	49.309893	8.499758	22.132940
C	49.200000	3.468530	3.690000	C	49.250163	10.696890	6.142490	C	49.450714	9.940342	22.155819
C	49.200000	6.360240	3.690000	C	49.276154	4.208112	7.373894	C	49.275569	2.026878	23.391156
C	49.200000	7.804660	3.690000	C	49.247415	5.652642	7.381951	C	49.234447	3.474103	23.366400
C	49.200000	10.697170	3.689980	C	49.251093	8.532987	7.372780	C	49.243224	6.347177	23.374935
C	49.200000	12.144060	3.690000	C	49.286832	9.975720	7.374022	C	49.297496	7.782100	23.364839
H	49.200000	13.991190	4.920000	C	49.446048	2.052307	8.610454	C	49.513876	10.653059	23.388164
H	49.200000	0.204130	4.920000	C	49.349630	3.506744	8.606657	C	49.232101	4.191706	24.603201
C	49.200000	1.312260	4.920000	C	49.242074	6.380194	8.609601	C	49.240164	5.633903	24.605696
C	49.200000	4.189910	4.920000	C	49.242471	7.821029	8.603421	C	49.321121	8.505032	24.602157
C	49.200000	5.636640	4.920000	C	49.359873	10.687607	8.601369	C	49.398114	9.944754	24.613327
C	49.200000	8.528800	4.920000	C	49.316927	4.236346	9.824688	C	49.231033	2.021872	25.837359
C	49.200000	9.973320	4.919980	C	49.226996	5.672325	9.851332	C	49.225189	3.475862	25.829657
C	49.200000	12.865540	4.920000	C	49.228004	8.545985	9.830196	C	49.236648	6.353191	25.834765
C	49.273620	12.156600	6.138320	C	49.311332	9.980989	9.839776	C	49.262089	7.795090	25.831876
H	49.454670	13.943780	7.368540	C	49.552830	2.091271	11.067819	C	49.352754	10.668204	25.835348
H	49.462080	0.239600	7.408120	C	49.359992	3.540045	11.062483	C	49.210150	4.191170	27.065255
C	49.390200	1.342450	7.389040	C	49.100642	6.396093	11.081671	C	49.212128	5.634753	27.064316
C	49.401410	12.839780	7.364590	C	49.106555	7.845572	11.067929	C	49.233360	8.522500	27.063120
C	49.456740	12.138450	8.585840	C	49.312905	10.706563	11.072137	C	49.250870	9.965850	27.066820
H	49.704110	13.927850	9.795670	C	49.189544	4.240752	12.267180	C	49.200000	2.010100	28.290000
H	49.730520	0.286090	9.855550	C	48.980387	5.662613	12.306777	C	49.200000	3.468530	28.290000
C	49.591880	1.382990	9.844470	C	49.000536	8.564354	12.280645	C	49.200000	6.360240	28.290000
C	49.588250	12.828480	9.801660	C	49.101376	9.998386	12.291061	C	49.200000	7.804660	28.290000
C	49.505580	12.157700	11.047560	N	49.540163	1.995683	13.491054	C	49.200000	10.697170	28.289980
H	49.711080	13.972540	12.181430	B	49.251717	3.435151	13.539149	C	49.200000	12.144060	28.290000
H	49.864260	0.299320	12.281930	N	48.666746	6.292216	13.508613	H	49.200000	13.991190	29.520000
C	49.668430	1.388530	12.279700	B	48.621794	7.775935	13.547229	H	49.200000	0.204130	29.520000
C	49.544850	12.880170	12.243280	N	49.013919	10.693823	13.495590	C	49.200000	1.312260	29.520000
B	49.272890	12.141390	13.528570	N	49.008994	4.083564	14.764246	C	49.200000	4.189910	29.520000
H	49.436250	13.803810	14.793620	B	48.523816	5.472115	14.757106	C	49.200000	5.636640	29.520000
H	49.933170	0.049210	14.676880	N	48.188577	8.606058	14.612679	C	49.200000	8.528800	29.520000
B	49.648310	1.238010	14.722690	B	48.613543	9.975142	14.724075	C	49.200000	9.973320	29.519980
N	49.219460	12.808740	14.784750	N	49.422188	1.924705	15.952885	C	49.200000	12.865540	29.520000
B	49.062720	12.106700	16.013300	B	49.078867	3.357024	15.993557	C	49.200000	2.010100	30.750000
H	49.523650	13.776660	17.233640	N	47.981591	5.991894	15.928850	C	49.200000	3.468530	30.750000
H	49.803640	-0.000240	17.180920	Cu	47.136242	7.821970	15.978532	C	49.200000	6.360240	30.750000
B	49.538060	1.193010	17.184620	N	48.700146	10.697720	15.983234	C	49.200000	7.804660	30.750000
N	49.292100	12.785590	17.255820	N	48.861607	4.049554	17.230719	C	49.200000	10.697170	30.749980
B	49.375920	12.058500	18.474230	B	48.420651	5.472695	17.164611	C	49.200000	12.144060	30.749990
H	49.857790	13.717010	19.745720	N	48.263523	8.621276	17.394604	H	49.200000	13.991190	31.980000
H	49.645360	-0.024400	19.663240	B	48.671265	9.963147	17.250813	H	49.200000	0.204130	31.980000
B	49.440040	1.183730	19.655020	N	49.352159	1.901677	18.422667	C	49.200000	1.312260	31.980000
N	49.706640	12.710180	19.709690	B	49.070373	3.338747	18.447696	C	49.200000	4.189910	31.980000
C	49.677860	12.067750	20.935750	N	48.525855	6.260491	18.414469	C	49.200000	5.636640	31.980000
H	49.927320	13.872910	22.129130	B	48.597539	7.747622	18.449857	C	49.200000	8.528800	31.979990
H	49.437940	0.229370	22.161100	N	49.120940	10.644084	18.450073	C	49.200382	9.975840	31.979151
C	49.340140	1.331190	22.157560	N	49.006988	4.094280	19.691208	C	49.200850	12.858614	31.979690

Cu/V_B-GBN + CO

C	49.200000	2.010100	1.230000	C	49.793680	12.775530	22.133850	B	48.879096	5.558366	19.630540
C	49.200000	3.468530	1.230000	C	49.657450	12.094280	23.375250	N	49.017966	8.436127	19.687224
C	49.200000	6.360240	1.230000	H	49.697590	13.896980	24.602020	B	49.210705	9.881174	19.650538
C	49.200000	7.804660	1.230000	H	49.284420	0.222840	24.605230	C	45.190236	7.895578	16.048550
C	49.200000	10.697170	1.229980	C	49.267400	1.327870	24.609650	O	44.028680	7.842616	16.045837
C	49.200000	12.144060	1.229990	C	49.611880	12.795220	24.600030	C	49.292485	2.001030	20.939406
H	49.200000	13.991190	2.460000	C	49.424730	12.118130	25.827600	C	49.151999	3.439305	20.912623
H	49.200000	0.204130	2.460000	H	49.350840	13.926650	27.045490	C	49.060862	6.346980	20.923161
C	49.200000	1.312260	2.460000	H	49.212090	0.214860	27.049890	C	49.127458	7.772763	20.901939
C	49.200000	4.189910	2.460000	C	49.213440	1.320630	27.059860	C	49.489771	10.645008	20.935815
C	49.200000	5.636640	2.460000	C	49.314500	12.821680	27.051510	C	49.163514	4.184013	22.132077
C	49.200000	8.528800	2.460000	C	49.264283	2.016483	6.151343	C	49.150162	5.635859	22.138366
C	49.200000	9.973320	2.459980	C	49.234910	3.475551	6.149639	C	49.290697	8.500494	22.128043
C	49.200000	12.865540	2.460000	C	49.206918	6.366260	6.147318	C	49.441918	9.940389	22.152294
C	49.200000	2.010100	3.690000	C	49.211054	7.807998	6.147769	C	49.269709	2.027111	23.388885
C	49.200000	3.468530	3.690000	C	49.248047	10.698823	6.143559	C	49.217659	3.472548	23.366325
C	49.200000	6.360240	3.690000	C	49.251671	4.208219	7.373919	C	49.221313	6.348029	23.374487
C	49.200000	7.804660	3.690000	C	49.220305	5.652703	7.382686	C	49.281536	7.782853	23.360226
C	49.200000	10.697170	3.689980	C	49.239979	8.533643	7.373563	C	49.509513	10.653704	23.384792
C	49.200000	12.144060	3.690000	C	49.281692	9.976243	7.374860	C	49.217077	4.192345	24.602784
H	49.200000	13.991190	4.920000	C	49.434751	2.052128	8.612384	C	49.223901	5.633932	24.605064
H	49.200000	0.204130	4.920000	C	49.316890	3.504882	8.606444	C	49.313597	8.506015	24.599461
C	49.200000	1.312260	4.920000	C	49.210391	6.380757	8.610531	C	49.393882	9.944783	24.610609
C	49.200000	4.189910	4.920000	C	49.228302	7.820781	8.606114	C	49.229334	2.022415	25.834955
C	49.200000	5.636640	4.920000	C	49.360440	10.689213	8.601959	C	49.218707	3.475399	25.829247
C	49.200000	8.528800	4.920000	C	49.267104	4.233397	9.824979	C	49.228726	6.354109	25.833820
C	49.200000	9.973320	4.919980	C	49.184352	5.670388	9.853264	C	49.255438	7.795563	25.829864
C	49.200000	12.865540	4.920000	C	49.233016	8.544515	9.834112	C	49.351769	10.668753	25.834220
C	49.273620	12.156600	6.138320	C	49.323794	9.978950	9.843579	C	49.207233	4.191915	27.063632
H	49.454670	13.943780	7.368540	C	49.535387	2.089161	11.070637	C	49.209164	5.634741	27.062901
H	49.462080	0.239600	7.408120	C	49.314087	3.535001	11.063254	C	49.230300	8.522724	27.061421
C	49.390200	1.342450	7.389040	C	49.075747	6.394130	11.083624	C	49.248316	9.964964	27.064592
C	49.401410	12.839780	7.364590	C	49.111088	7.842697	11.071939	C	49.200000	2.010100	28.290000
C	49.456740	12.138450	8.585840	C	49.334726	10.705187	11.072544	C	49.200000	3.468530	28.290000
H	49.704110	13.927850	9.795670	C	49.139995	4.235952	12.267686	C	49.200000	6.360240	28.290000
H	49.730520	0.286090	9.855550	C	48.943990	5.660378	12.311393	C	49.200000	7.804660	28.290000
C	49.591880	1.382990	9.844470	C	49.013268	8.563368	12.285302	C	49.200000	10.697170	28.289980
C	49.588250	12.828480	9.801660	C	49.128497	9.994218	12.295414	C	49.200000	12.144060	28.290000
C	49.505580	12.157700	11.047560	N	49.532044	1.997191	13.495105	H	49.200000	13.991190	29.520000
H	49.711080	13.972540	12.181430	B	49.222363	3.432302	13.542226	H	49.200000	0.204130	29.520000
H	49.864260	0.299320	12.281930	N	48.649908	6.291890	13.513009	C	49.200000	1.312260	29.520000
C	49.668430	1.388530	12.279700	B	48.634053	7.780487	13.562935	C	49.200000	4.189910	29.520000
C	49.544850	12.880170	12.243280	N	49.034142	10.696042	13.493787	C	49.200000	5.636640	29.520000
B	49.272890	12.141390	13.528570	N	48.993736	4.085816	14.768336	C	49.200000	8.528800	29.520000
H	49.436250	13.803810	14.793620	B	48.529492	5.483011	14.770836	C	49.200000	9.973320	29.519980
H	49.933170	0.049210	14.676880	N	48.258640	8.609335	14.641173	C	49.200000	12.865540	29.520000
B	49.648310	1.238010	14.722690	B	48.642291	9.974932	14.724016	C	49.200000	2.010100	30.750000
N	49.219460	12.808740	14.784750	N	49.423778	1.924759	15.954722	C	49.200000	3.468530	30.750000
B	49.062720	12.106700	16.013300	B	49.083409	3.356797	15.994568	C	49.200000	6.360240	30.750000
H	49.523650	13.776660	17.233640	N	48.037921	6.025208	15.957098	C	49.200000	7.804660	30.750000
H	49.803640	-0.000240	17.180920	Cu	47.065224	7.775779	16.005262	C	49.200000	10.697170	30.749980
B	49.538060	1.193010	17.184620	N	48.712971	10.702088	15.981097	C	49.200000	12.144060	30.749990
N	49.292100	12.785590	17.255820	N	48.885529	4.047648	17.234158	H	49.200000	13.991190	31.980000
B	49.375920	12.058500	18.474230	B	48.463314	5.470868	17.175058	H	49.200000	0.204130	31.980000
H	49.857790	13.717010	19.745720	N	48.304861	8.586779	17.352075	C	49.200000	1.312260	31.980000
H	49.645360	-0.024400	19.663240	B	48.679708	9.949554	17.232675	C	49.200000	4.189910	31.980000
B	49.440040	1.183730	19.655020	N	49.355097	1.899078	18.424253	C	49.200000	5.636640	31.980000
N	49.706640	12.710180	19.709690	B	49.081920	3.335229	18.449347	C	49.200000	8.528800	31.979990
C	49.677860	12.067750	20.935750	N	48.582641	6.252977	18.416857	C	49.200000	9.973320	31.979980
H	49.927320	13.872910	22.129130	B	48.617762	7.728638	18.433529	C	49.200000	12.865540	31.980000
H	49.437940	0.229370	22.161100	N	49.104777	10.639294	18.444647				
C	49.340140	1.331190	22.157560	N	49.014846	4.090144	19.693512				

Cu/V_B-GBN + PH₃

C	49.200000	2.010100	1.230000	C	49.793680	12.775530	22.133850	B	48.868667	5.560888	19.632774
C	49.200000	3.468530	1.230000	C	49.657450	12.094280	23.375250	N	49.011673	8.437652	19.695855
C	49.200000	6.360240	1.230000	H	49.697590	13.896980	24.602020	B	49.206440	9.883392	19.655023
C	49.200000	7.804660	1.230000	H	49.284420	0.222840	24.605230	P	44.864244	8.016394	15.551614
C	49.200000	10.697170	1.229980	C	49.267400	1.327870	24.609650	H	44.358148	9.095064	14.726330
C	49.200000	12.144060	1.229990	C	49.611880	12.795220	24.600030	H	44.172075	6.963399	14.833204
H	49.200000	13.991190	2.460000	C	49.424730	12.118130	25.827600	H	43.844462	8.150631	16.572929
H	49.200000	0.204130	2.460000	H	49.350840	13.926650	27.045490	C	49.292842	2.001221	20.940656
C	49.200000	1.312260	2.460000	H	49.212090	0.214860	27.049890	C	49.150935	3.441093	20.914542
C	49.200000	4.189910	2.460000	C	49.213440	1.320630	27.059860	C	49.053210	6.346995	20.927499
C	49.200000	5.636640	2.460000	C	49.314500	12.821680	27.051510	C	49.120888	7.773920	20.909725
C	49.200000	8.528800	2.460000	C	49.265029	2.014005	6.149692	C	49.483367	10.644688	20.938051
C	49.200000	9.973320	2.459980	C	49.237954	3.475000	6.150177	C	49.164292	4.184267	22.134380
C	49.200000	12.865540	2.460000	C	49.208501	6.365268	6.145418	C	49.148383	5.636445	22.141923
C	49.200000	2.010100	3.690000	C	49.209716	7.807284	6.145054	C	49.285220	8.500038	22.133483
C	49.200000	3.468530	3.690000	C	49.246385	10.697244	6.142606	C	49.437670	9.939870	22.155593
C	49.200000	6.360240	3.690000	C	49.255720	4.206946	7.372868	C	49.270433	2.026360	23.391898
C	49.200000	7.804660	3.690000	C	49.222933	5.651887	7.380904	C	49.220583	3.473225	23.369215
C	49.200000	10.697170	3.689980	C	49.233619	8.532745	7.371154	C	49.221185	6.347887	23.378791
C	49.200000	12.144060	3.690000	C	49.276157	9.975910	7.373331	C	49.277094	7.782899	23.366077
H	49.200000	13.991190	4.920000	C	49.434189	2.051323	8.610255	C	49.506676	10.652431	23.386598
H	49.200000	0.204130	4.920000	C	49.317768	3.504702	8.606196	C	49.222318	4.191499	24.605390
C	49.200000	1.312260	4.920000	C	49.207447	6.378677	8.607525	C	49.228626	5.633841	24.608356
C	49.200000	4.189910	4.920000	C	49.220049	7.819737	8.601338	C	49.310357	8.505331	24.602589
C	49.200000	5.636640	4.920000	C	49.355626	10.687254	8.600858	C	49.389777	9.944736	24.613403
C	49.200000	8.528800	4.920000	C	49.262925	4.231949	9.823179	C	49.230786	2.021953	25.837760
C	49.200000	9.973320	4.919980	C	49.177686	5.669264	9.849975	C	49.223150	3.475398	25.831386
C	49.200000	12.865540	4.920000	C	49.223445	8.543422	9.828063	C	49.234156	6.353119	25.836419
C	49.273620	12.156600	6.138320	C	49.316274	9.979040	9.839257	C	49.258167	7.794894	25.832954
H	49.454670	13.943780	7.368540	C	49.532902	2.090416	11.067296	C	49.350862	10.668029	25.835178
H	49.462080	0.239600	7.408120	C	49.306520	3.535276	11.061161	C	49.210894	4.190902	27.065791
C	49.390200	1.342450	7.389040	C	49.064591	6.392626	11.080202	C	49.213234	5.634482	27.065356
C	49.401410	12.839780	7.364590	C	49.107655	7.842400	11.066586	C	49.233360	8.522500	27.063120
C	49.456740	12.138450	8.585840	C	49.330401	10.704224	11.070041	C	49.250870	9.965850	27.066820
H	49.704110	13.927850	9.795670	C	49.125052	4.234774	12.264790	C	49.200000	2.010100	28.290000
H	49.730520	0.286090	9.855550	C	48.928022	5.659573	12.307665	C	49.200000	3.468530	28.290000
C	49.591880	1.382990	9.844470	C	49.028853	8.559885	12.280220	C	49.200000	6.360240	28.290000
C	49.588250	12.828480	9.801660	C	49.138580	9.993918	12.292878	C	49.200000	7.804660	28.290000
C	49.505580	12.157700	11.047560	N	49.526914	1.995762	13.488928	C	49.200000	10.697170	28.289980
H	49.711080	13.972540	12.181430	B	49.206940	3.433498	13.539200	C	49.200000	12.144060	28.290000
H	49.864260	0.299320	12.281930	N	48.632714	6.290606	13.510097	H	49.200000	13.991190	29.520000
C	49.668430	1.388530	12.279700	B	48.634437	7.782221	13.553417	H	49.200000	0.204130	29.520000
C	49.544850	12.880170	12.243280	N	49.052966	10.692119	13.493832	C	49.200000	1.312260	29.520000
B	49.272890	12.141390	13.528570	N	48.971396	4.083010	14.765013	C	49.200000	4.189910	29.520000
H	49.436250	13.803810	14.793620	B	48.499558	5.481618	14.769678	C	49.200000	5.636640	29.520000
H	49.933170	0.049210	14.676880	N	48.243341	8.613701	14.618317	C	49.200000	8.528800	29.520000
B	49.648310	1.238010	14.722690	B	48.644604	9.970374	14.721706	C	49.200000	9.973320	29.519980
N	49.219460	12.808740	14.784750	N	49.420501	1.925138	15.951895	C	49.200000	12.865540	29.520000
B	49.062720	12.106700	16.013300	B	49.069626	3.357675	15.994357	C	49.200000	2.010100	30.750000
H	49.523650	13.776660	17.233640	N	47.998645	6.015149	15.956527	C	49.200000	3.468530	30.750000
H	49.803640	-0.000240	17.180920	Cu	47.076797	7.801807	16.001988	C	49.200000	6.360240	30.750000
B	49.538060	1.193010	17.184620	N	48.701426	10.699011	15.983225	C	49.200000	7.804660	30.750000
N	49.292100	12.785590	17.255820	N	48.871600	4.048271	17.234395	C	49.200000	10.697170	30.749980
B	49.375920	12.058500	18.474230	B	48.439296	5.473756	17.176300	C	49.200000	12.144060	30.749990
H	49.857790	13.717010	19.745720	N	48.231707	8.601734	17.384894	H	49.200000	13.991190	31.980000
H	49.645360	-0.024400	19.663240	B	48.654501	9.951641	17.242819	H	49.200000	0.204130	31.980000
B	49.440040	1.183730	19.655020	N	49.353610	1.899787	18.423345	C	49.200000	1.312260	31.980000
N	49.706640	12.710180	19.709690	B	49.075479	3.336983	18.449504	C	49.200000	4.189910	31.980000
C	49.677860	12.067750	20.935750	N	48.561519	6.256059	18.419717	C	49.200000	5.636640	31.980000
H	49.927320	13.872910	22.129130	B	48.586448	7.737699	18.447657	C	49.200000	8.528800	31.979990
H	49.437940	0.229370	22.161100	N	49.108503	10.638755	18.445299	C	49.200195	9.975672	31.979490
C	49.340140	1.331190	22.157560	N	49.009770	4.091251	19.695112	C	49.200774	12.858546	31.979700

Cu/V_B-GBN + HCN

C	49.200000	2.010100	1.230000	C	49.793680	12.775530	22.133850	B	48.884728	5.566988	19.639826
C	49.200000	3.468530	1.230000	C	49.657450	12.094280	23.375250	N	49.027000	8.444331	19.708346
C	49.200000	6.360240	1.230000	H	49.697590	13.896980	24.602020	B	49.216984	9.888152	19.660563
C	49.200000	7.804660	1.230000	H	49.284420	0.222840	24.605230	C	45.107230	7.840974	16.418565
C	49.200000	10.697170	1.229980	C	49.267400	1.327870	24.609650	N	45.139114	7.276419	15.348482
C	49.200000	12.144060	1.229990	C	49.611880	12.795220	24.600030	H	44.529834	8.241352	17.267798
H	49.200000	13.991190	2.460000	C	49.424730	12.118130	25.827600	C	49.298178	2.002018	20.940761
H	49.200000	0.204130	2.460000	H	49.350840	13.926650	27.045490	C	49.164857	3.442897	20.915099
C	49.200000	1.312260	2.460000	H	49.212090	0.214860	27.049890	C	49.082510	6.351274	20.932733
C	49.200000	4.189910	2.460000	C	49.213440	1.320630	27.059860	C	49.154399	7.778412	20.915149
C	49.200000	5.636640	2.460000	C	49.314500	12.821680	27.051510	C	49.497255	10.645535	20.942159
C	49.200000	8.528800	2.460000	C	49.263843	2.014052	6.150235	C	49.182216	4.185718	22.135592
C	49.200000	9.973320	2.459980	C	49.236137	3.475017	6.150140	C	49.176865	5.638593	22.144014
C	49.200000	12.865540	2.460000	C	49.213341	6.366556	6.144136	C	49.325915	8.501508	22.138684
C	49.200000	2.010100	3.690000	C	49.218289	7.808609	6.144711	C	49.465713	9.940671	22.158661
C	49.200000	3.468530	3.690000	C	49.249288	10.697787	6.142617	C	49.271352	2.026408	23.392175
C	49.200000	6.360240	3.690000	C	49.260296	4.208081	7.370732	C	49.225768	3.473935	23.369526
C	49.200000	7.804660	3.690000	C	49.235186	5.653322	7.378004	C	49.247866	6.349145	23.381167
C	49.200000	10.697170	3.689980	C	49.252997	8.534885	7.369904	C	49.313169	7.783774	23.368801
C	49.200000	12.144060	3.690000	C	49.288386	9.977161	7.373577	C	49.525755	10.652541	23.389900
H	49.200000	13.991190	4.920000	C	49.437693	2.051346	8.609732	C	49.218517	4.192442	24.606024
H	49.200000	0.204130	4.920000	C	49.330343	3.505200	8.603479	C	49.233986	5.634816	24.609321
C	49.200000	1.312260	4.920000	C	49.239752	6.381236	8.603379	C	49.335896	8.505897	24.605309
C	49.200000	4.189910	4.920000	C	49.253560	7.821941	8.599255	C	49.410783	9.944926	24.615278
C	49.200000	5.636640	4.920000	C	49.367034	10.688268	8.601283	C	49.226097	2.022194	25.838149
C	49.200000	8.528800	4.920000	C	49.299049	4.233697	9.818893	C	49.212549	3.475961	25.831284
C	49.200000	9.973320	4.919980	C	49.225783	5.671497	9.844256	C	49.233135	6.354287	25.837456
C	49.200000	12.865540	4.920000	C	49.262792	8.545786	9.825369	C	49.266620	7.795792	25.833928
C	49.273620	12.156600	6.138320	C	49.339687	9.980839	9.839998	C	49.356820	10.668432	25.836410
H	49.454670	13.943780	7.368540	C	49.544970	2.089811	11.065878	C	49.202213	4.191312	27.065736
H	49.462080	0.239600	7.408120	C	49.346765	3.536283	11.056422	C	49.205798	5.634956	27.065037
C	49.390200	1.342450	7.389040	C	49.132154	6.395512	11.072907	C	49.234850	8.522791	27.063700
C	49.401410	12.839780	7.364590	C	49.162740	7.844551	11.062489	C	49.250870	9.965850	27.066820
C	49.456740	12.138450	8.585840	C	49.344480	10.705620	11.071484	C	49.200000	2.010100	28.290000
H	49.704110	13.927850	9.795670	C	49.193773	4.237154	12.261135	C	49.200000	3.468530	28.290000
H	49.730520	0.286090	9.855550	C	49.017774	5.662066	12.299696	C	49.200000	6.360240	28.290000
C	49.591880	1.382990	9.844470	C	49.083613	8.562386	12.274960	C	49.200000	7.804660	28.290000
C	49.588250	12.828480	9.801660	C	49.161650	9.996224	12.295150	C	49.200000	10.697170	28.289980
C	49.505580	12.157700	11.047560	N	49.532847	1.995062	13.488177	C	49.200000	12.144060	28.290000
H	49.711080	13.972540	12.181430	B	49.248081	3.437229	13.536842	H	49.200000	13.991190	29.520000
H	49.864260	0.299320	12.281930	N	48.751064	6.297195	13.499088	H	49.200000	0.204130	29.520000
C	49.668430	1.388530	12.279700	B	48.709502	7.782840	13.544409	C	49.200000	1.312260	29.520000
C	49.544850	12.880170	12.243280	N	49.060006	10.688125	13.498417	C	49.200000	4.189910	29.520000
B	49.272890	12.141390	13.528570	N	49.026031	4.091111	14.763111	C	49.200000	5.636640	29.520000
H	49.436250	13.803810	14.793620	B	48.624513	5.506204	14.753855	C	49.200000	8.528800	29.520000
H	49.933170	0.049210	14.676880	N	48.281788	8.583378	14.610595	C	49.200000	9.973320	29.519980
B	49.648310	1.238010	14.722690	B	48.656267	9.954870	14.731156	C	49.200000	12.865540	29.520000
N	49.219460	12.808740	14.784750	N	49.428733	1.929477	15.952482	C	49.200000	2.010100	30.750000
B	49.062720	12.106700	16.013300	B	49.099421	3.368856	15.996128	C	49.200000	3.468530	30.750000
H	49.523650	13.776660	17.233640	N	48.179920	6.072205	15.942843	C	49.200000	6.360240	30.750000
H	49.803640	-0.000240	17.180920	Cu	47.100969	7.781334	15.994463	C	49.200000	7.804660	30.750000
B	49.538060	1.193010	17.184620	N	48.692419	10.691792	15.990034	C	49.200000	10.697170	30.749980
N	49.292100	12.785590	17.255820	N	48.901492	4.064218	17.234857	C	49.200000	12.144060	30.749990
B	49.375920	12.058500	18.474230	B	48.514829	5.506639	17.185033	H	49.200000	13.991190	31.980000
H	49.857790	13.717010	19.745720	N	48.154229	8.614708	17.426669	H	49.200000	0.204130	31.980000
H	49.645360	-0.024400	19.663240	B	48.618937	9.948953	17.263236	C	49.200000	1.312260	31.980000
B	49.440040	1.183730	19.655020	N	49.351001	1.901973	18.422968	C	49.200000	4.189910	31.980000
N	49.706640	12.710180	19.709690	B	49.085828	3.343087	18.450228	C	49.200000	5.636640	31.980000
C	49.677860	12.067750	20.935750	N	48.569505	6.270264	18.435510	C	49.200000	8.528800	31.979990
H	49.927320	13.872910	22.129130	B	48.559829	7.759357	18.470909	C	49.200000	9.973320	31.979980
H	49.437940	0.229370	22.161100	N	49.110396	10.639696	18.450579	C	49.201067	12.858334	31.979903
C	49.340140	1.331190	22.157560	N	49.026073	4.094984	19.696572				

Cu/V_{B+N}-GBN + NO₂

C	49.200000	2.010100	1.230000	C	49.200077	12.884619	22.176162	N	49.063624	8.490824	19.750660
C	49.200000	3.468530	1.230000	C	49.199944	12.175614	23.406925	B	49.137072	9.943764	19.696502
C	49.200000	6.360240	1.230000	H	49.199841	13.968468	24.651859	C	49.182891	2.023369	20.956498
C	49.200000	7.804660	1.230000	H	49.199986	0.230153	24.608907	N	45.930907	6.120544	16.477593
C	49.200000	10.697170	1.229980	C	49.199990	1.335254	24.618497	O	46.781895	5.288799	17.088160
C	49.200000	12.144060	1.229990	C	49.199951	12.863389	24.632031	O	46.431468	7.122757	15.958828
H	49.200000	13.991190	2.460000	C	49.200073	12.155402	25.850059	C	49.159922	3.468965	20.931140
H	49.200000	0.204130	2.460000	H	49.199843	13.952998	27.086771	C	49.181049	6.391426	20.954499
C	49.200000	1.312260	2.460000	H	49.199799	0.216524	27.050764	C	49.169632	7.821659	20.951843
C	49.200000	4.189910	2.460000	C	49.199947	1.321395	27.063427	C	49.207598	10.733715	20.984313
C	49.200000	5.636640	2.460000	C	49.200004	12.848194	27.073815	C	49.220822	4.211624	22.148459
C	49.200000	8.528800	2.460000	C	49.201778	2.014636	6.147894	C	49.241261	5.666995	22.160847
C	49.200000	9.973320	2.459980	C	49.206138	3.472443	6.146013	C	49.239965	8.555837	22.171508
C	49.200000	12.865540	2.460000	C	49.211669	6.365360	6.142644	C	49.227277	10.009379	22.189719
C	49.200000	2.010100	3.690000	C	49.209548	7.807078	6.141760	C	49.210994	2.041116	23.401404
C	49.200000	3.468530	3.690000	C	49.200315	10.703167	6.136459	C	49.234732	3.489636	23.377161
C	49.200000	6.360240	3.690000	C	49.225187	4.201393	7.369085	C	49.271993	6.378183	23.395653
C	49.200000	7.804660	3.690000	C	49.233542	5.648341	7.373117	C	49.269137	7.819513	23.388767
C	49.200000	10.697170	3.689980	C	49.222724	8.539780	7.359669	C	49.223935	10.722020	23.417042
C	49.200000	12.144060	3.690000	C	49.210786	9.984704	7.363471	C	49.245360	4.206650	24.611983
H	49.200000	13.991190	4.920000	C	49.210541	2.029078	8.607000	C	49.260803	5.650799	24.616913
H	49.200000	0.204130	4.920000	C	49.234659	3.489060	8.596953	C	49.255727	8.539876	24.621634
C	49.200000	1.312260	4.920000	C	49.266835	6.382063	8.591280	C	49.232334	9.985964	24.630735
C	49.200000	4.189910	4.920000	C	49.257245	7.826162	8.583502	C	49.207215	2.028776	25.841805
C	49.200000	5.636640	4.920000	C	49.214883	10.713018	8.581646	C	49.222798	3.482613	25.833938
C	49.200000	8.528800	4.920000	C	49.270717	4.223152	9.812377	C	49.242016	6.367364	25.843185
C	49.200000	9.973320	4.919980	C	49.299377	5.666852	9.826598	C	49.240025	7.811190	25.841016
C	49.200000	12.865540	4.920000	C	49.279630	8.564083	9.798390	C	49.212817	10.701105	25.851944
C	49.200068	12.159323	6.130012	C	49.246741	10.005221	9.817984	C	49.212862	4.196119	27.067016
H	49.199819	13.965642	7.334810	C	49.218654	2.058299	11.063588	C	49.216789	5.639077	27.065776
H	49.199837	0.219973	7.388993	C	49.262231	3.517984	11.045288	C	49.214708	8.531661	27.069059
C	49.199927	1.324994	7.380722	C	49.339212	6.404278	11.044537	C	49.209587	9.974133	27.070534
C	49.199997	12.861304	7.344847	C	49.332385	7.858640	11.026868	C	49.200000	2.010100	28.290000
C	49.199963	12.166760	8.564240	C	49.244262	10.742821	11.038956	C	49.200000	3.468530	28.290000
H	49.199843	13.983617	9.748425	C	49.282492	4.242435	12.249334	C	49.200000	6.360240	28.290000
H	49.199885	0.236157	9.849808	C	49.327122	5.666596	12.265253	C	49.200000	7.804660	28.290000
C	49.199911	1.341621	9.839439	C	49.355606	8.588044	12.228922	C	49.200000	10.697170	28.289980
C	49.199891	12.878818	9.770707	C	49.294961	10.016096	12.265520	C	49.200000	12.144060	28.290000
C	49.200117	12.205753	11.013245	N	49.201523	2.018783	13.497859	H	49.200000	13.991190	29.520000
H	49.200043	14.028479	12.142825	B	49.207651	3.482218	13.545680	H	49.200000	0.204130	29.520000
H	49.200645	0.266559	12.314367	N	49.311464	6.321937	13.480845	C	49.200000	1.312260	29.520000
C	49.201131	1.372206	12.287684	B	49.383308	7.793680	13.519932	C	49.200000	4.189910	29.520000
C	49.200371	12.923536	12.212965	N	49.266758	10.681208	13.484714	C	49.200000	5.636640	29.520000
B	49.201532	12.147729	13.509101	N	49.095189	4.193293	14.781510	C	49.200000	8.528800	29.520000
H	49.200993	13.818601	14.778304	B	49.086881	5.638285	14.753925	C	49.200000	9.973320	29.519980
H	49.200738	0.045677	14.696438	N	49.414601	8.488468	14.722238	C	49.200000	12.865540	29.520000
B	49.202291	1.267445	14.730561	B	49.279957	9.900562	14.751671	C	49.200000	2.010100	30.750000
N	49.202015	12.800794	14.774715	N	49.171026	1.989312	15.959594	C	49.200000	3.468530	30.750000
B	49.202554	12.086353	16.009377	B	49.030068	3.445287	16.011741	C	49.200000	6.360240	30.750000
H	49.200686	13.821095	17.232154	Cu	48.700320	7.165084	15.996246	C	49.200000	7.804660	30.750000
H	49.200673	0.027277	17.167480	N	49.157467	10.645775	15.983478	C	49.200000	10.697170	30.749980
B	49.202473	1.247654	17.186090	N	48.864403	4.125524	17.249464	C	49.200000	12.144060	30.749990
N	49.201959	12.803053	17.254317	B	48.309429	5.509797	17.270128	H	49.200000	13.991190	31.980000
B	49.202106	12.101354	18.491813	N	48.663845	8.547125	17.338724	H	49.200000	0.204130	31.980000
H	49.200263	13.821866	19.778895	B	48.984250	9.916707	17.228481	C	49.200000	1.312260	31.980000
H	49.200358	-0.004112	19.647603	N	49.195439	1.952046	18.432730	C	49.200000	4.189910	31.980000
B	49.201551	1.220151	19.657215	B	49.042098	3.399741	18.461972	C	49.200000	5.636640	31.980000
N	49.200891	12.803338	19.747650	N	48.666678	6.311338	18.477816	C	49.200000	8.528800	31.979990
C	49.200474	12.172625	20.977818	B	48.779228	7.775179	18.502050	C	49.200000	9.973320	31.979980
H	49.200185	13.990479	22.188290	N	49.125455	10.664623	18.468648	C	49.200000	12.865540	31.980000
H	49.199942	0.235072	22.179306	N	49.052664	4.133955	19.717701				
C	49.200154	1.340855	22.172715	B	48.992499	5.600593	19.668676				

Cu/V_{B+N}-GBN + CO

C	49.200000	2.010100	1.230000	C	49.200077	12.884619	22.176162	N	49.394311	8.491983	19.744772
C	49.200000	3.468530	1.230000	C	49.199944	12.175614	23.406925	B	49.312851	9.945779	19.688655
C	49.200000	6.360240	1.230000	H	49.199841	13.968468	24.651859	C	49.218427	2.022558	20.955495
C	49.200000	7.804660	1.230000	H	49.199986	0.230153	24.608907	C	46.344993	7.139741	16.123592
C	49.200000	10.697170	1.229980	C	49.199990	1.335254	24.618497	O	45.212597	7.150048	15.870707
C	49.200000	12.144060	1.229990	C	49.199951	12.863389	24.632031	C	49.264571	3.464310	20.933701
H	49.200000	13.991190	2.460000	C	49.200073	12.155402	25.850059	C	49.384968	6.388611	20.957286
H	49.200000	0.204130	2.460000	H	49.199843	13.952998	27.086771	C	49.381067	7.821713	20.949656
C	49.200000	1.312260	2.460000	H	49.199799	0.216524	27.050764	C	49.263350	10.734182	20.980971
C	49.200000	4.189910	2.460000	C	49.199947	1.321395	27.063427	C	49.283625	4.209617	22.148560
C	49.200000	5.636640	2.460000	C	49.200004	12.848194	27.073815	C	49.322612	5.665523	22.163202
C	49.200000	8.528800	2.460000	C	49.203088	2.014930	6.148255	C	49.315490	8.555875	22.170178
C	49.200000	9.973320	2.459980	C	49.209757	3.472901	6.147021	C	49.268202	10.009372	22.186892
C	49.200000	12.865540	2.460000	C	49.220854	6.365126	6.144207	C	49.212430	2.041079	23.400156
C	49.200000	2.010100	3.690000	C	49.219760	7.806870	6.142021	C	49.242376	3.488616	23.378201
C	49.200000	3.468530	3.690000	C	49.205338	10.703222	6.136038	C	49.281528	6.378561	23.396831
C	49.200000	6.360240	3.690000	C	49.230574	4.202106	7.371505	C	49.277624	7.819335	23.387842
C	49.200000	7.804660	3.690000	C	49.243141	5.649247	7.376754	C	49.221808	10.721652	23.414999
C	49.200000	10.697170	3.689980	C	49.240789	8.539772	7.359673	C	49.232025	4.206820	24.612734
C	49.200000	12.144060	3.690000	C	49.225746	9.984222	7.362025	C	49.241077	5.651260	24.617299
H	49.200000	13.991190	4.920000	C	49.210083	2.029905	8.607502	C	49.232247	8.540208	24.620335
H	49.200000	0.204130	4.920000	C	49.232381	3.490534	8.599927	C	49.216792	9.986229	24.629375
C	49.200000	1.312260	4.920000	C	49.268532	6.382879	8.597913	C	49.203058	2.028483	25.840994
C	49.200000	4.189910	4.920000	C	49.270405	7.826597	8.585362	C	49.209962	3.482634	25.834021
C	49.200000	5.636640	4.920000	C	49.229213	10.713040	8.580224	C	49.217544	6.368216	25.843063
C	49.200000	8.528800	4.920000	C	49.244078	4.226088	9.817952	C	49.214964	7.811649	25.840225
C	49.200000	9.973320	4.919980	C	49.264983	5.669736	9.837952	C	49.202085	10.701163	25.851274
C	49.200000	12.865540	4.920000	C	49.284574	8.564568	9.799865	C	49.203491	4.196406	27.067255
C	49.200068	12.159323	6.130012	C	49.258561	10.005654	9.815173	C	49.204534	5.639111	27.065762
H	49.199819	13.965642	7.334810	C	49.205905	2.060620	11.065210	C	49.202418	8.532093	27.068840
H	49.199837	0.219973	7.388993	C	49.215694	3.523439	11.050815	C	49.200682	9.974301	27.070331
C	49.199927	1.324994	7.380722	C	49.252304	6.408297	11.061231	C	49.200000	2.010100	28.290000
C	49.199997	12.861304	7.344847	C	49.281102	7.861503	11.032084	C	49.200000	3.468530	28.290000
C	49.199963	12.166760	8.564240	C	49.233777	10.744479	11.035248	C	49.200000	6.360240	28.290000
H	49.199843	13.983617	9.748425	C	49.168513	4.250775	12.256435	C	49.200000	7.804660	28.290000
H	49.199885	0.236157	9.849808	C	49.168737	5.677376	12.289957	C	49.200000	10.697170	28.289980
C	49.199911	1.341621	9.839439	C	49.247531	8.591448	12.232636	C	49.200000	12.144060	28.290000
C	49.199891	12.878818	9.770707	C	49.217163	10.021039	12.260693	H	49.200000	13.991190	29.520000
C	49.200117	12.205753	11.013245	N	49.175997	2.019468	13.500741	H	49.200000	0.204130	29.520000
H	49.200043	14.028479	12.142825	B	49.106124	3.482311	13.544913	C	49.200000	1.312260	29.520000
H	49.200645	0.266559	12.314367	N	49.046059	6.339035	13.507372	C	49.200000	4.189910	29.520000
C	49.201131	1.372206	12.287684	B	49.001752	7.819888	13.512659	C	49.200000	5.636640	29.520000
C	49.200371	12.923536	12.212965	N	49.155845	10.686164	13.475768	C	49.200000	8.528800	29.520000
B	49.201532	12.147729	13.509101	N	48.984768	4.191061	14.780942	C	49.200000	9.973320	29.519980
H	49.200993	13.818601	14.778304	B	48.895399	5.641524	14.793451	C	49.200000	12.865540	29.520000
H	49.200738	0.045677	14.696438	N	48.647736	8.522405	14.650978	C	49.200000	2.010100	30.750000
B	49.202291	1.267445	14.730561	B	48.941651	9.908252	14.726952	C	49.200000	3.468530	30.750000
N	49.202015	12.800794	14.774715	N	49.164723	1.990790	15.960118	C	49.200000	6.360240	30.750000
B	49.202554	12.086353	16.009377	B	49.054797	3.444139	16.000096	C	49.200000	7.804660	30.750000
H	49.200686	13.821095	17.232154	Cu	48.284711	7.143749	16.038758	C	49.200000	10.697170	30.749980
H	49.200673	0.027277	17.167480	N	49.066856	10.645876	15.973135	C	49.200000	12.144060	30.749990
B	49.202473	1.247654	17.186090	N	49.065231	4.165183	17.237267	H	49.200000	13.991190	31.980000
N	49.201959	12.803053	17.254317	B	49.035705	5.623578	17.186254	H	49.200000	0.204130	31.980000
B	49.202106	12.101354	18.491813	N	49.059525	8.481389	17.307964	C	49.200000	1.312260	31.980000
H	49.200263	13.821866	19.778895	B	49.112807	9.889939	17.216502	C	49.200000	4.189910	31.980000
H	49.200358	-0.004112	19.647603	N	49.201347	1.958480	18.430068	C	49.200000	5.636640	31.980000
B	49.201551	1.220151	19.657215	B	49.187154	3.414616	18.460040	C	49.200000	8.528800	31.979990
N	49.200891	12.803338	19.747650	N	49.315902	6.300009	18.428642	C	49.200000	9.973320	31.979980
C	49.200474	12.172625	20.977818	B	49.280672	7.771334	18.474338	C	49.200000	12.865540	31.980000
H	49.200185	13.990479	22.188290	N	49.243096	10.658668	18.457515				
H	49.199942	0.235072	22.179306	N	49.275899	4.133474	19.712771				
C	49.200154	1.340855	22.172715	B	49.355864	5.589840	19.664740				

Cu/V_{B+N}-GBN + NH₃

C	49.200000	2.010100	1.230000	C	49.200077	12.884619	22.176162	N	49.344774	8.492916	19.754823
C	49.200000	3.468530	1.230000	C	49.199944	12.175614	23.406925	B	49.286654	9.946700	19.694468
C	49.200000	6.360240	1.230000	H	49.199841	13.968468	24.651859	C	49.214494	2.020630	20.957148
C	49.200000	7.804660	1.230000	H	49.199986	0.230153	24.608907	N	46.134058	7.493837	16.261989
C	49.200000	10.697170	1.229980	C	49.199990	1.335254	24.618497	H	45.670469	7.274713	17.152239
C	49.200000	12.144060	1.229990	C	49.199951	12.863389	24.632031	H	45.512730	7.167678	15.512224
H	49.200000	13.991190	2.460000	C	49.200073	12.155402	25.850059	H	46.175594	8.517842	16.188714
H	49.200000	0.204130	2.460000	H	49.199843	13.952998	27.086771	C	49.253242	3.463131	20.938970
C	49.200000	1.312260	2.460000	H	49.199799	0.216524	27.050764	C	49.365872	6.388115	20.969340
C	49.200000	4.189910	2.460000	C	49.199947	1.321395	27.063427	C	49.364054	7.821598	20.960370
C	49.200000	5.636640	2.460000	C	49.200004	12.848194	27.073815	C	49.262445	10.733958	20.984473
C	49.200000	8.528800	2.460000	C	49.200626	2.011600	6.147220	C	49.285786	4.207948	22.153547
C	49.200000	9.973320	2.459980	C	49.203616	3.471623	6.147392	C	49.328950	5.664218	22.172756
C	49.200000	12.865540	2.460000	C	49.211148	6.364340	6.141086	C	49.326602	8.555911	22.176596
C	49.200000	2.010100	3.690000	C	49.210653	7.807115	6.139475	C	49.276690	10.009522	22.190314
C	49.200000	3.468530	3.690000	C	49.200645	10.701728	6.134437	C	49.214991	2.039564	23.403611
C	49.200000	6.360240	3.690000	C	49.218314	4.200991	7.369445	C	49.249843	3.488474	23.383111
C	49.200000	7.804660	3.690000	C	49.229385	5.648610	7.373281	C	49.301245	6.378412	23.404629
C	49.200000	10.697170	3.689980	C	49.227399	8.539213	7.357559	C	49.296929	7.819989	23.395598
C	49.200000	12.144060	3.690000	C	49.215557	9.984110	7.360992	C	49.229758	10.720954	23.417798
H	49.200000	13.991190	4.920000	C	49.206216	2.028213	8.606021	C	49.241904	4.205947	24.616341
H	49.200000	0.204130	4.920000	C	49.224029	3.489845	8.598427	C	49.254971	5.651073	24.622981
C	49.200000	1.312260	4.920000	C	49.260324	6.381387	8.591176	C	49.244006	8.539612	24.624203
C	49.200000	4.189910	4.920000	C	49.263154	7.826567	8.580808	C	49.223798	9.986587	24.632508
C	49.200000	5.636640	4.920000	C	49.226096	10.711326	8.578402	C	49.203636	2.027726	25.844077
C	49.200000	8.528800	4.920000	C	49.242216	4.224197	9.812261	C	49.213990	3.482691	25.837201
C	49.200000	9.973320	4.919980	C	49.266169	5.668437	9.828413	C	49.223538	6.367761	25.846600
C	49.200000	12.865540	4.920000	C	49.289351	8.564026	9.793710	C	49.219538	7.811625	25.843728
C	49.200068	12.159323	6.130012	C	49.262188	10.005901	9.811150	C	49.201778	10.700473	25.852674
H	49.199819	13.965642	7.334810	C	49.207609	2.060242	11.061722	C	49.204921	4.195678	27.069822
H	49.199837	0.219973	7.388993	C	49.218219	3.521690	11.046409	C	49.205900	5.639261	27.068998
C	49.199927	1.324994	7.380722	C	49.261824	6.406595	11.047743	C	49.201063	8.531834	27.070772
C	49.199997	12.861304	7.344847	C	49.295265	7.860938	11.025840	C	49.198020	9.975070	27.072631
C	49.199963	12.166760	8.564240	C	49.241319	10.743424	11.032843	C	49.200000	2.010100	28.290000
H	49.199843	13.983617	9.748425	C	49.167700	4.247800	12.248056	C	49.200000	3.468530	28.290000
H	49.199885	0.236157	9.849808	C	49.165423	5.675749	12.270762	C	49.200000	6.360240	28.290000
C	49.199911	1.341621	9.839439	C	49.267041	8.589053	12.225454	C	49.200000	7.804660	28.290000
C	49.199891	12.878818	9.770707	C	49.232788	10.021087	12.256015	C	49.200000	10.697170	28.289980
C	49.200117	12.205753	11.013245	N	49.174049	2.017296	13.493859	C	49.200000	12.144060	28.290000
H	49.200043	14.028479	12.142825	B	49.099857	3.484355	13.538901	H	49.200000	13.991190	29.520000
H	49.200645	0.266559	12.314367	N	49.022051	6.335759	13.477510	H	49.200000	0.204130	29.520000
C	49.201131	1.372206	12.287684	B	49.002845	7.819546	13.500486	C	49.200000	1.312260	29.520000
C	49.200371	12.923536	12.212965	N	49.167536	10.685271	13.472291	C	49.200000	4.189910	29.520000
B	49.201532	12.147729	13.509101	N	48.961713	4.189252	14.771221	C	49.200000	5.636640	29.520000
H	49.200993	13.818601	14.778304	B	48.848940	5.641066	14.760085	C	49.200000	8.528800	29.520000
H	49.200738	0.045677	14.696438	N	48.651065	8.519109	14.644855	C	49.200000	9.973320	29.519980
B	49.202291	1.267445	14.730561	B	48.953453	9.902593	14.722052	C	49.200000	12.865540	29.520000
N	49.202015	12.800794	14.774715	N	49.161486	1.993740	15.957657	C	49.200000	2.010100	30.750000
B	49.202554	12.086353	16.009377	B	49.034388	3.451815	15.998909	C	49.200000	3.468530	30.750000
H	49.200686	13.821095	17.232154	Cu	48.414063	7.108149	16.010294	C	49.200000	6.360240	30.750000
H	49.200673	0.027277	17.167480	N	49.066315	10.642340	15.972416	C	49.200000	7.804660	30.750000
B	49.202473	1.247654	17.186090	N	49.029200	4.165501	17.241811	C	49.200000	10.697170	30.749980
N	49.201959	12.803053	17.254317	B	48.965228	5.627953	17.210230	C	49.200000	12.144060	30.749990
B	49.202106	12.101354	18.491813	N	48.956095	8.485725	17.326857	H	49.200000	13.991190	31.980000
H	49.200263	13.821866	19.778895	B	49.072984	9.890938	17.222931	H	49.200000	0.204130	31.980000
H	49.200358	-0.004112	19.647603	N	49.196014	1.958103	18.429971	C	49.200000	1.312260	31.980000
B	49.201551	1.220151	19.657215	B	49.161753	3.415039	18.463069	C	49.200000	4.189910	31.980000
N	49.200891	12.803338	19.747650	N	49.215688	6.301014	18.458764	C	49.200000	5.636640	31.980000
C	49.200474	12.172625	20.977818	B	49.188194	7.772676	18.492899	C	49.200000	8.528800	31.979990
H	49.200185	13.990479	22.188290	N	49.216688	10.659200	18.460847	C	49.200000	9.973320	31.979980
H	49.199942	0.235072	22.179306	N	49.241584	4.131253	19.719454	C	49.200000	12.865540	31.980000
C	49.200154	1.340855	22.172715	B	49.300296	5.589013	19.682930				

Cu/V_{B+N}-GBN + PH₃

C	49.200000	2.010100	1.230000	C	49.200077	12.884619	22.176162	N	49.339894	8.492155	19.755761
C	49.200000	3.468530	1.230000	C	49.199944	12.175614	23.406925	B	49.281214	9.946074	19.694395
C	49.200000	6.360240	1.230000	H	49.199841	13.968468	24.651859	C	49.216773	2.021075	20.957261
C	49.200000	7.804660	1.230000	H	49.199986	0.230153	24.608907	P	46.051445	7.520290	16.220411
C	49.200000	10.697170	1.229980	C	49.199990	1.335254	24.618497	H	45.236391	7.238998	17.386775
C	49.200000	12.144060	1.229990	C	49.199951	12.863389	24.632031	H	45.016115	7.122622	15.284947
H	49.200000	13.991190	2.460000	C	49.200073	12.155402	25.850059	H	45.707945	8.925737	16.180478
H	49.200000	0.204130	2.460000	H	49.199843	13.952998	27.086771	C	49.255731	3.463803	20.938718
C	49.200000	1.312260	2.460000	H	49.199799	0.216524	27.050764	C	49.346588	6.387173	20.968153
C	49.200000	4.189910	2.460000	C	49.199947	1.321395	27.063427	C	49.341920	7.820759	20.960410
C	49.200000	5.636640	2.460000	C	49.200004	12.848194	27.073815	C	49.248848	10.733177	20.984074
C	49.200000	8.528800	2.460000	C	49.207426	2.011778	6.146710	C	49.278086	4.207901	22.153838
C	49.200000	9.973320	2.459980	C	49.220705	3.471807	6.146761	C	49.310418	5.664113	22.172115
C	49.200000	12.865540	2.460000	C	49.239156	6.364822	6.140855	C	49.298160	8.554685	22.177125
C	49.200000	2.010100	3.690000	C	49.235140	7.807483	6.138966	C	49.257245	10.008591	22.190145
C	49.200000	3.468530	3.690000	C	49.208827	10.701787	6.134686	C	49.213761	2.039449	23.403667
C	49.200000	6.360240	3.690000	C	49.259856	4.200898	7.368900	C	49.246314	3.488451	23.382924
C	49.200000	7.804660	3.690000	C	49.278786	5.648513	7.372247	C	49.288496	6.377032	23.405339
C	49.200000	10.697170	3.689980	C	49.264471	8.539837	7.356459	C	49.281531	7.818596	23.395320
C	49.200000	12.144060	3.690000	C	49.237722	9.984136	7.360840	C	49.223240	10.720626	23.418227
H	49.200000	13.991190	4.920000	C	49.220176	2.028405	8.605815	C	49.245975	4.205495	24.616983
H	49.200000	0.204130	4.920000	C	49.263117	3.489747	8.598266	C	49.260895	5.650429	24.623168
C	49.200000	1.312260	4.920000	C	49.316686	6.381148	8.589789	C	49.251975	8.538924	24.625312
C	49.200000	4.189910	4.920000	C	49.309961	7.826675	8.579038	C	49.229390	9.986057	24.632485
C	49.200000	5.636640	4.920000	C	49.239069	10.711539	8.577467	C	49.206333	2.027548	25.843986
C	49.200000	8.528800	4.920000	C	49.289262	4.224085	9.812086	C	49.221130	3.482197	25.837040
C	49.200000	9.973320	4.919980	C	49.320981	5.668556	9.827734	C	49.243036	6.367353	25.847524
C	49.200000	12.865540	4.920000	C	49.323480	8.564766	9.790757	C	49.241345	7.811258	25.843929
C	49.200068	12.159323	6.130012	C	49.280235	10.006193	9.809785	C	49.212652	10.700914	25.853249
H	49.199819	13.965642	7.334810	C	49.218476	2.060349	11.061497	C	49.212353	4.195596	27.069777
H	49.199837	0.219973	7.388993	C	49.254416	3.521686	11.045725	C	49.218786	5.639332	27.069209
C	49.199927	1.324994	7.380722	C	49.316771	6.406891	11.047412	C	49.217494	8.531853	27.071085
C	49.199997	12.861304	7.344847	C	49.335852	7.861513	11.022053	C	49.210620	9.975373	27.072717
C	49.199963	12.166760	8.564240	C	49.250088	10.744179	11.031234	C	49.200000	2.010100	28.290000
H	49.199843	13.983617	9.748425	C	49.223296	4.248220	12.247726	C	49.200000	3.468530	28.290000
H	49.199885	0.236157	9.849808	C	49.238408	5.675554	12.272285	C	49.200000	6.360240	28.290000
C	49.199911	1.341621	9.839439	C	49.308360	8.590776	12.220140	C	49.200000	7.804660	28.290000
C	49.199891	12.878818	9.770707	C	49.254175	10.022059	12.254210	C	49.200000	10.697170	28.289980
C	49.200117	12.205753	11.013245	N	49.187245	2.017604	13.493645	C	49.200000	12.144060	28.290000
H	49.200043	14.028479	12.142825	B	49.146693	3.485233	13.537860	H	49.200000	13.991190	29.520000
H	49.200645	0.266559	12.314367	N	49.120921	6.334816	13.483917	H	49.200000	0.204130	29.520000
C	49.201131	1.372206	12.287684	B	49.092489	7.815355	13.498182	C	49.200000	1.312260	29.520000
C	49.200371	12.923536	12.212965	N	49.186644	10.686008	13.470746	C	49.200000	4.189910	29.520000
B	49.201532	12.147729	13.509101	N	49.026848	4.190544	14.771879	C	49.200000	5.636640	29.520000
H	49.200993	13.818601	14.778304	B	48.935673	5.642049	14.766278	C	49.200000	8.528800	29.520000
H	49.200738	0.045677	14.696438	N	48.760471	8.509730	14.647225	C	49.200000	9.973320	29.519980
B	49.202291	1.267445	14.730561	B	49.001188	9.902489	14.722774	C	49.200000	12.865540	29.520000
N	49.202015	12.800794	14.774715	N	49.168409	1.992393	15.957675	C	49.200000	2.010100	30.750000
B	49.202554	12.086353	16.009377	B	49.064961	3.450522	15.998262	C	49.200000	3.468530	30.750000
H	49.200686	13.821095	17.232154	Cu	48.413819	7.117175	16.004184	C	49.200000	6.360240	30.750000
H	49.200673	0.027277	17.167480	N	49.081169	10.642846	15.972916	C	49.200000	7.804660	30.750000
B	49.202473	1.247654	17.186090	N	49.051492	4.164956	17.239456	C	49.200000	10.697170	30.749980
N	49.201959	12.803053	17.254317	B	48.995029	5.626045	17.202413	C	49.200000	12.144060	30.749990
B	49.202106	12.101354	18.491813	N	48.983885	8.485444	17.326334	H	49.200000	13.991190	31.980000
H	49.200263	13.821866	19.778895	B	49.088664	9.891871	17.222586	H	49.200000	0.204130	31.980000
H	49.200358	-0.004112	19.647603	N	49.199554	1.958354	18.429594	C	49.200000	1.312260	31.980000
B	49.201551	1.220151	19.657215	B	49.173612	3.415072	18.462470	C	49.200000	4.189910	31.980000
N	49.200891	12.803338	19.747650	N	49.244518	6.300921	18.450941	C	49.200000	5.636640	31.980000
C	49.200474	12.172625	20.977818	B	49.208027	7.771131	18.492397	C	49.200000	8.528800	31.979990
H	49.200185	13.990479	22.188290	N	49.224217	10.659090	18.460539	C	49.200000	9.973320	31.979980
H	49.199942	0.235072	22.179306	N	49.252890	4.131310	19.718571	C	49.200000	12.865540	31.980000
C	49.200154	1.340855	22.172715	B	49.308361	5.588607	19.679323				

Cu/V_{B+N}-GBN + HCN

C	49.200000	2.010100	1.230000	C	49.200077	12.884619	22.176162	N	48.984700	8.493786	19.758895
C	49.200000	3.468530	1.230000	C	49.199944	12.175614	23.406925	B	49.082888	9.945616	19.694746
C	49.200000	6.360240	1.230000	H	49.199841	13.968468	24.651859	C	49.176518	2.021497	20.958293
C	49.200000	7.804660	1.230000	H	49.199986	0.230153	24.608907	C	46.028462	7.461583	15.918387
C	49.200000	10.697170	1.229980	C	49.199990	1.335254	24.618497	N	45.111616	6.858671	15.499398
C	49.200000	12.144060	1.229990	C	49.199951	12.863389	24.632031	H	46.914413	7.993052	16.328245
H	49.200000	13.991190	2.460000	C	49.200073	12.155402	25.850059	C	49.119780	3.463155	20.943541
H	49.200000	0.204130	2.460000	H	49.199843	13.952998	27.086771	C	49.021593	6.388744	20.981040
C	49.200000	1.312260	2.460000	H	49.199799	0.216524	27.050764	C	49.043510	7.821168	20.964961
C	49.200000	4.189910	2.460000	C	49.199947	1.321395	27.063427	C	49.162988	10.732664	20.984034
C	49.200000	5.636640	2.460000	C	49.200004	12.848194	27.073815	C	49.132863	4.208066	22.158054
C	49.200000	8.528800	2.460000	C	49.199972	2.011614	6.146926	C	49.108162	5.663958	22.180288
C	49.200000	9.973320	2.459980	C	49.200820	3.470979	6.146233	C	49.132085	8.554872	22.177569
C	49.200000	12.865540	2.460000	C	49.205144	6.364696	6.139468	C	49.165455	10.009308	22.189987
C	49.200000	2.010100	3.690000	C	49.203809	7.807366	6.138330	C	49.193893	2.039616	23.404105
C	49.200000	3.468530	3.690000	C	49.200106	10.701995	6.134614	C	49.178047	3.488290	23.385562
C	49.200000	6.360240	3.690000	C	49.209615	4.200157	7.367303	C	49.162356	6.378811	23.409171
C	49.200000	7.804660	3.690000	C	49.214895	5.647986	7.369783	C	49.166335	7.819403	23.397061
C	49.200000	10.697170	3.689980	C	49.211391	8.539967	7.355546	C	49.193930	10.721498	23.418315
C	49.200000	12.144060	3.690000	C	49.203763	9.984557	7.360939	C	49.191140	4.206193	24.618380
H	49.200000	13.991190	4.920000	C	49.204809	2.027894	8.605211	C	49.190233	5.650971	24.626580
H	49.200000	0.204130	4.920000	C	49.217871	3.488828	8.595770	C	49.193236	8.540300	24.625543
C	49.200000	1.312260	4.920000	C	49.237902	6.380819	8.585364	C	49.197268	9.986825	24.632809
C	49.200000	4.189910	4.920000	C	49.230721	7.826767	8.577384	C	49.199518	2.027308	25.844334
C	49.200000	5.636640	4.920000	C	49.203078	10.711949	8.577409	C	49.199596	3.482410	25.838124
C	49.200000	8.528800	4.920000	C	49.255941	4.222969	9.807540	C	49.200448	6.368919	25.848789
C	49.200000	9.973320	4.919980	C	49.274769	5.667206	9.819711	C	49.201036	7.812043	25.844946
C	49.200000	12.865540	4.920000	C	49.243194	8.564500	9.789300	C	49.200474	10.701133	25.853091
C	49.200068	12.159323	6.130012	C	49.219877	10.005943	9.810414	C	49.200924	4.196228	27.070196
H	49.199819	13.965642	7.334810	C	49.221736	2.059545	11.060675	C	49.202172	5.639617	27.069701
H	49.199837	0.219973	7.388993	C	49.273618	3.519582	11.041252	C	49.201066	8.532309	27.071728
C	49.199927	1.324994	7.380722	C	49.334184	6.405723	11.034607	C	49.200650	9.975165	27.073099
C	49.199997	12.861304	7.344847	C	49.302080	7.860844	11.017908	C	49.200000	2.010100	28.290000
C	49.199963	12.166760	8.564240	C	49.227296	10.743387	11.031644	C	49.200000	3.468530	28.290000
H	49.199843	13.983617	9.748425	C	49.353679	4.244935	12.240635	C	49.200000	6.360240	28.290000
H	49.199885	0.236157	9.849808	C	49.400978	5.671427	12.252571	C	49.200000	7.804660	28.290000
C	49.199911	1.341621	9.839439	C	49.342493	8.589450	12.215438	C	49.200000	10.697170	28.289980
C	49.199891	12.878818	9.770707	C	49.289116	10.020154	12.254130	C	49.200000	12.144060	28.290000
C	49.200117	12.205753	11.013245	N	49.235414	2.019050	13.493264	H	49.200000	13.991190	29.520000
H	49.200043	14.028479	12.142825	B	49.331697	3.484095	13.536158	H	49.200000	0.204130	29.520000
H	49.200645	0.266559	12.314367	N	49.522636	6.331906	13.459808	C	49.200000	1.312260	29.520000
C	49.201131	1.372206	12.287684	B	49.547156	7.817723	13.498521	C	49.200000	4.189910	29.520000
C	49.200371	12.923536	12.212965	N	49.295098	10.684616	13.473450	C	49.200000	5.636640	29.520000
B	49.201532	12.147729	13.509101	N	49.374396	4.196096	14.773852	C	49.200000	8.528800	29.520000
H	49.200993	13.818601	14.778304	B	49.481357	5.641689	14.743974	C	49.200000	9.973320	29.519980
H	49.200738	0.045677	14.696438	N	49.732426	8.514103	14.689201	C	49.200000	12.865540	29.520000
B	49.202291	1.267445	14.730561	B	49.429573	9.901123	14.733356	C	49.200000	2.010100	30.750000
N	49.202015	12.800794	14.774715	N	49.210675	1.996636	15.958054	C	49.200000	3.468530	30.750000
B	49.202554	12.086353	16.009377	B	49.236947	3.461598	16.000178	C	49.200000	6.360240	30.750000
H	49.200686	13.821095	17.232154	Cu	49.374377	7.136004	16.005151	C	49.200000	7.804660	30.750000
H	49.200673	0.027277	17.167480	N	49.230200	10.635905	15.974758	C	49.200000	10.697170	30.749980
B	49.202473	1.247654	17.186090	N	49.115708	4.172904	17.241454	C	49.200000	12.144060	30.749990
N	49.201959	12.803053	17.254317	B	49.040308	5.629746	17.227322	H	49.200000	13.991190	31.980000
B	49.202106	12.101354	18.491813	N	48.799380	8.493760	17.297330	H	49.200000	0.204130	31.980000
H	49.200263	13.821866	19.778895	B	49.053697	9.895082	17.215691	C	49.200000	1.312260	31.980000
H	49.200358	-0.004112	19.647603	N	49.179051	1.959414	18.430574	C	49.200000	4.189910	31.980000
B	49.201551	1.220151	19.657215	B	49.101082	3.414106	18.466260	C	49.200000	5.636640	31.980000
N	49.200891	12.803338	19.747650	N	48.842351	6.299887	18.480124	C	49.200000	8.528800	31.979990
C	49.200474	12.172625	20.977818	B	48.853914	7.775357	18.497411	C	49.200000	9.973320	31.979980
H	49.200185	13.990479	22.188290	N	49.116657	10.658185	18.459976	C	49.200000	12.865540	31.980000
H	49.199942	0.235072	22.179306	N	49.044917	4.130118	19.725586				
C	49.200154	1.340855	22.172715	B	48.945873	5.585573	19.702266				

Cu/V_{B+N}-GBN

C	49.200000	2.010100	1.230000	H	49.200043	14.028479	12.142825	C	49.200077	12.884619	22.176162
C	49.200000	3.468530	1.230000	H	49.200645	0.266559	12.314367	C	49.200011	2.039232	23.404693
C	49.200000	6.360240	1.230000	C	49.201131	1.372206	12.287684	C	49.200050	3.487684	23.390717
C	49.200000	7.804660	1.230000	C	49.201088	4.242322	12.231903	C	49.199921	6.380713	23.421270
C	49.200000	10.697170	1.229980	C	49.201175	5.668516	12.234537	C	49.199921	7.821776	23.409526
C	49.200000	12.144060	1.229990	C	49.201022	8.592398	12.189255	C	49.199917	10.723223	23.424284
H	49.200000	13.991190	2.460000	C	49.201135	10.022058	12.244545	C	49.199944	12.175614	23.406925
H	49.200000	0.204130	2.460000	C	49.200371	12.923536	12.212965	H	49.199841	13.968468	24.651859
C	49.200000	1.312260	2.460000	N	49.202533	2.017604	13.492627	H	49.199986	0.230153	24.608907
C	49.200000	4.189910	2.460000	B	49.202416	3.484346	13.529423	C	49.199990	1.335254	24.618497
C	49.200000	5.636640	2.460000	N	49.202272	6.329788	13.436300	C	49.199989	4.206162	24.623044
C	49.200000	8.528800	2.460000	B	49.202366	7.809685	13.468338	C	49.199936	5.651877	24.634316
C	49.200000	9.973320	2.459980	N	49.202198	10.685688	13.464796	C	49.199954	8.543049	24.634214
C	49.200000	12.865540	2.460000	B	49.201532	12.147729	13.509101	C	49.200004	9.988873	24.638446
C	49.200000	2.010100	3.690000	H	49.200993	13.818601	14.778304	C	49.199951	12.863389	24.632031
C	49.200000	3.468530	3.690000	H	49.200738	0.045677	14.696438	C	49.200001	2.027245	25.843913
C	49.200000	6.360240	3.690000	B	49.202291	1.267445	14.730561	C	49.200029	3.481564	25.840343
C	49.200000	7.804660	3.690000	N	49.203158	4.198431	14.764559	C	49.200034	6.370313	25.854451
C	49.200000	10.697170	3.689980	B	49.202289	5.647993	14.723048	C	49.200064	7.813953	25.850705
C	49.200000	12.144060	3.690000	N	49.203839	8.494106	14.664870	C	49.200138	10.702479	25.856181
H	49.200000	13.991190	4.920000	B	49.203255	9.901075	14.726346	C	49.200073	12.155402	25.850059
H	49.200000	0.204130	4.920000	N	49.202015	12.800794	14.774715	H	49.199843	13.952998	27.086771
C	49.200000	1.312260	4.920000	N	49.203327	1.998574	15.958082	H	49.199799	0.216524	27.050764
C	49.200000	4.189910	4.920000	B	49.203477	3.464755	16.000105	C	49.199947	1.321395	27.063427
C	49.200000	5.636640	4.920000	Cu	49.201168	7.116861	15.990019	C	49.200051	4.195334	27.071722
C	49.200000	8.528800	4.920000	N	49.203587	10.641178	15.976599	C	49.200066	5.638993	27.072192
C	49.200000	9.973320	4.919980	B	49.202554	12.086353	16.009377	C	49.200127	8.534499	27.074646
C	49.200000	12.865540	4.920000	H	49.200686	13.821095	17.232154	C	49.200143	9.976803	27.074946
C	49.200018	2.010773	6.146500	H	49.200673	0.027277	17.167480	C	49.200004	12.848194	27.073815
C	49.200037	3.469924	6.144125	B	49.202473	1.247654	17.186090	C	49.200000	2.010100	28.290000
C	49.200051	6.365308	6.136374	N	49.203606	4.173881	17.248695	C	49.200000	3.468530	28.290000
C	49.200094	7.807147	6.134728	B	49.202789	5.633588	17.246554	C	49.200000	6.360240	28.290000
C	49.200100	10.703495	6.132536	N	49.203254	8.483047	17.338941	C	49.200000	7.804660	28.290000
C	49.200068	12.159323	6.130012	B	49.203471	9.891386	17.226779	C	49.200000	10.697170	28.289980
H	49.199819	13.965642	7.334810	N	49.201959	12.803053	17.254317	C	49.200000	12.144060	28.290000
H	49.199837	0.219973	7.388993	N	49.203206	1.958464	18.431494	H	49.200000	13.991190	29.520000
C	49.199927	1.324994	7.380722	B	49.203318	3.415780	18.472493	H	49.200000	0.204130	29.520000
C	49.199992	4.199418	7.363369	N	49.203786	6.302429	18.510010	C	49.200000	1.312260	29.520000
C	49.199994	5.646999	7.363497	B	49.203304	7.772918	18.527303	C	49.200000	4.189910	29.520000
C	49.200117	8.541825	7.348369	N	49.203426	10.660270	18.469011	C	49.200000	5.636640	29.520000
C	49.200110	9.986121	7.356335	B	49.202106	12.101354	18.491813	C	49.200000	8.528800	29.520000
C	49.199997	12.861304	7.344847	H	49.200263	13.821866	19.778895	C	49.200000	9.973320	29.519980
C	49.199896	2.026867	8.604645	H	49.200358	-0.004112	19.647603	C	49.200000	12.865540	29.520000
C	49.199959	3.486986	8.590621	B	49.201551	1.220151	19.657215	C	49.200000	2.010100	30.750000
C	49.199921	6.381175	8.575609	N	49.202616	4.130006	19.734353	C	49.200000	3.468530	30.750000
C	49.199978	7.826674	8.566021	B	49.202668	5.586578	19.722396	C	49.200000	6.360240	30.750000
C	49.200009	10.713128	8.572386	N	49.202700	8.497043	19.783873	C	49.200000	7.804660	30.750000
C	49.199963	12.166760	8.564240	B	49.202296	9.949079	19.705374	C	49.200000	10.697170	30.749980
H	49.199843	13.983617	9.748425	N	49.200891	12.803338	19.747650	C	49.200000	12.144060	30.749990
H	49.199885	0.236157	9.849808	C	49.200850	2.020143	20.959246	H	49.200000	13.991190	31.980000
C	49.199911	1.341621	9.839439	C	49.201260	3.462104	20.950279	H	49.200000	0.204130	31.980000
C	49.200006	4.221217	9.800528	C	49.201254	6.391487	20.997838	C	49.200000	1.312260	31.980000
C	49.199970	5.665601	9.807130	C	49.201353	7.824426	20.983614	C	49.200000	4.189910	31.980000
C	49.199993	8.566178	9.774195	C	49.200704	10.735369	20.992207	C	49.200000	5.636640	31.980000
C	49.200041	10.007185	9.802531	C	49.200474	12.172625	20.977818	C	49.200000	8.528800	31.979990
C	49.199891	12.878818	9.770707	H	49.200185	13.990479	22.188290	C	49.200000	9.973320	31.979980
C	49.200373	2.057958	11.059808	H	49.199942	0.235072	22.179306	C	49.200000	12.865540	31.980000
C	49.200396	3.517062	11.033528	C	49.200154	1.340855	22.172715				
C	49.200315	6.405323	11.017783	C	49.200427	4.208415	22.164964				
C	49.200284	7.860479	10.997638	C	49.200386	5.665382	22.193370				
C	49.200303	10.745404	11.023585	C	49.200325	8.559507	22.193984				
C	49.200117	12.205753	11.013245	C	49.200216	10.012249	22.199345				