Structure and Bonding in the Omnicapped Truncated Tetrahedral Au_{20} Cluster: Analogies between Gold and Carbon Cluster Chemistry

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Supporting Information

S-Table 1 Total energies (au), Number of Imaginary frequencies and Zero-Point Energies (au) of M_{20} clusters

	Symm	E_{tot}	NImag	ZPE
Cu_{20}	T_d	-3923.80211	0	0.01533
	C_{2v}	-3923.79612	0	0.01507
	C_s	-3923.80147	1	0.01510
	C_1	-3923.80280	0	0.01512
Ag_{20}	T_d	-2916.24337	0	0.01055
	C_{2v}	-2916.19935	0	0.00996
	C_s	-2916.22307	1	0.01031
	C_1	-2916.22388	0	0.01042
Au_{20}	T_d	-2710.10810	0	0.00896
	C_s	-2710.04459	0	0.00843
Li_{20}	T_d	-150.52485	0	0.02390
	C_{2v}	-150.56182	0	0.02518
Na_{20}	T_d	-3246.20278	0	0.00972
	C_{2v}	-3246.19796	0	0.01020
	C_s	-3246.20415	0	0.00998
K_{20}	T_d	-563.01958	0	0.00545
	C_{2v}	-563.01243	0	0.00541
	C_s	-563.01798	0	0.00541
Rb_{20}	T_d	-477.55523	0	0.00320
	C_{2v}	-477.54204	0	0.00312
	C_s	-477.55127	0	0.00321
Cs_{20}	T_d	-397.78006	0	0.00222
	C_{2v}	-397.76781	1	0.00215
	C_s	-397.76782	0	0.00216
	C_s	-397.77649	0	0.002217

S-Figure 1. Optimized structures and their Cartesian coordinates**Cu₂₀ (*T_d*)**

Cu	0.960470	0.960470	0.960470
Cu	-0.960470	-0.960470	0.960470
Cu	-0.960470	0.960470	-0.960470
Cu	0.960470	-0.960470	-0.960470
Cu	2.724202	0.880682	-0.880682
Cu	-2.724202	-0.880682	-0.880682
Cu	-0.880682	2.724202	0.880682
Cu	0.880682	-2.724202	0.880682
Cu	-2.724202	0.880682	0.880682
Cu	2.724202	-0.880682	0.880682
Cu	-0.880682	-2.724202	-0.880682
Cu	0.880682	2.724202	-0.880682
Cu	-0.880682	-0.880682	-2.724202
Cu	0.880682	0.880682	-2.724202
Cu	0.880682	-0.880682	2.724202
Cu	-0.880682	0.880682	2.724202
Cu	2.635520	2.635520	-2.635520
Cu	-2.635520	-2.635520	-2.635520
Cu	-2.635520	2.635520	2.635520
Cu	2.635520	-2.635520	2.635520

Cu	-1.412865	2.028294	-2.125769
Cu	1.412865	2.028294	-2.125769
Cu	1.412865	2.028294	2.125769
Cu	-1.412865	2.028294	2.125769
Cu	0.000000	-2.095199	2.022718
Cu	0.000000	-2.095199	-2.022718
Cu	-2.246516	-0.489062	-2.099647
Cu	2.246516	-0.489062	-2.099647
Cu	2.246516	-0.489062	2.099647
Cu	-2.246516	-0.489062	2.099647
Cu	2.257789	0.914100	0.000000
Cu	-2.257789	0.914100	0.000000
Cu	1.466675	-1.629547	0.000000
Cu	-1.466675	-1.629547	0.000000
Cu	0.000000	2.446800	0.000000
Cu	0.000000	-3.687629	0.000000
Cu	0.000000	0.131656	-3.523347
Cu	0.000000	0.131656	3.523347
Cu	0.000000	0.220941	-1.193490
Cu	0.000000	0.220941	1.193490

Cu₂₀ (C_s)

Cu	-1.829447	-2.020184	0.000000
Cu	-0.179441	1.888590	1.300874
Cu	1.859706	-1.632802	-2.274093
Cu	-0.677206	3.940425	0.000000
Cu	-2.346166	1.876706	0.000000
Cu	-1.836430	-0.026518	1.553595
Cu	2.104874	0.796755	1.376588
Cu	2.104874	0.796755	-1.376588
Cu	-3.767103	-0.380658	0.000000
Cu	-0.585695	-2.128176	-2.187186
Cu	0.251456	0.106809	2.976168
Cu	0.265683	-0.358346	0.000000
Cu	-0.179441	1.888590	-1.300874
Cu	0.666485	-2.748711	0.000000
Cu	1.698473	2.938487	0.000000
Cu	-0.585695	-2.128176	2.187186
Cu	-1.836430	-0.026518	-1.553595
Cu	1.859706	-1.632802	2.274093
Cu	0.251456	0.106809	-2.976168
Cu	2.760338	-1.257033	0.000000

Cu₂₀ (C₁)

Cu	-2.467323	-1.154854	-0.014383
Cu	0.574303	1.843359	1.318057
Cu	1.068912	-2.232350	-2.287543
Cu	0.903980	3.891131	-0.037235
Cu	-1.432525	2.635514	-0.003370
Cu	-1.738506	0.707615	1.575052
Cu	2.294982	-0.063437	1.396386
Cu	2.204541	-0.100350	-1.358058
Cu	-3.618875	1.107439	-0.017452
Cu	-1.381328	-1.731644	-2.229199
Cu	0.269877	0.007253	2.968135
Cu	0.105375	-0.438624	0.198050
Cu	0.559818	1.782944	-1.283428
Cu	-0.448152	-2.783220	-0.081559
Cu	2.704669	2.049949	-0.017993
Cu	-1.353532	-1.741503	2.155816
Cu	-1.671919	0.665781	-1.534366
Cu	1.096714	-2.219116	2.267273
Cu	0.276063	0.001086	-3.003186
Cu	2.052926	-2.226974	-0.010997

Ag₂₀ (T_d)

Ag	1.121351	1.121351	1.121351
Ag	-1.121351	-1.121351	1.121351
Ag	-1.121351	1.121351	-1.121351
Ag	1.121351	-1.121351	-1.121351
Ag	3.129019	0.992034	-0.992034
Ag	-3.129019	-0.992034	-0.992034
Ag	-0.992034	3.129019	0.992034
Ag	0.992034	-3.129019	0.992034
Ag	-3.129019	0.992034	0.992034
Ag	3.129019	-0.992034	0.992034
Ag	-0.992034	-3.129019	-0.992034
Ag	0.992034	3.129019	-0.992034
Ag	-0.992034	-0.992034	-3.129019
Ag	0.992034	0.992034	-3.129019
Ag	0.992034	-0.992034	3.129019
Ag	-0.992034	0.992034	3.129019
Ag	2.994355	2.994355	-2.994355
Ag	-2.994355	-2.994355	-2.994355
Ag	-2.994355	2.994355	2.994355
Ag	2.994355	-2.994355	2.994355

Ag₂₀ (C_{2v})

Ag	-1.594402	2.318224	-2.446948
Ag	1.594402	2.318224	-2.446948
Ag	1.594402	2.318224	2.446948
Ag	-1.594402	2.318224	2.446948
Ag	0.000000	-2.395968	2.287922
Ag	0.000000	-2.395968	-2.287922
Ag	-2.564799	-0.523703	-2.414254
Ag	2.564799	-0.523703	-2.414254
Ag	2.564799	-0.523703	2.414254
Ag	-2.564799	-0.523703	2.414254
Ag	2.605568	1.075739	0.000000
Ag	-2.605568	1.075739	0.000000
Ag	1.790585	-1.877872	0.000000
Ag	-1.790585	-1.877872	0.000000
Ag	0.000000	2.790149	0.000000
Ag	0.000000	-4.174501	0.000000
Ag	0.000000	0.065304	-4.031181
Ag	0.000000	0.065304	4.031181
Ag	0.000000	0.235931	-1.340436
Ag	0.000000	0.235931	1.340436

Ag₂₀ (C_s)

Ag	-2.072951	-2.257709	0.000000
Ag	-0.223462	2.173756	1.584243
Ag	2.172014	-1.892479	-2.640201
Ag	-0.758095	4.467974	0.000000
Ag	-2.618341	2.077423	0.000000
Ag	-2.130672	-0.039153	1.917799
Ag	2.391648	0.896273	1.563105
Ag	2.391648	0.896273	-1.563105
Ag	-4.262895	-0.405300	0.000000
Ag	-0.649793	-2.457102	-2.521054
Ag	0.325762	0.094436	3.443946
Ag	0.169821	-0.278226	0.000000
Ag	-0.223462	2.173756	-1.584243
Ag	0.732649	-3.047105	0.000000
Ag	1.920130	3.330792	0.000000
Ag	-0.649793	-2.457102	2.521054
Ag	-2.130672	-0.039153	-1.917799
Ag	2.172014	-1.892479	2.640201
Ag	0.325762	0.094436	-3.443946
Ag	3.118687	-1.439311	0.000000

$\text{Ag}_{20} (C_1)$

Ag	-2.858846	-1.194350	-0.048172
Ag	0.712807	2.112506	1.566913
Ag	1.125845	-2.626467	-2.585299
Ag	1.162970	4.383581	-0.086364
Ag	-1.532911	2.989135	0.015219
Ag	-2.005883	0.828856	1.940925
Ag	2.603381	-0.138135	1.584037
Ag	2.492939	-0.249267	-1.475247
Ag	-4.053538	1.412614	0.046247
Ag	-1.724183	-1.886492	-2.759947
Ag	0.313558	0.012348	3.417067
Ag	0.027178	-0.389596	0.217952
Ag	0.692468	2.010730	-1.536250
Ag	-0.739937	-3.101856	-0.355198
Ag	3.145356	2.238631	-0.045527
Ag	-1.355174	-2.042998	2.309974
Ag	-1.901616	0.834556	-1.864252
Ag	1.455760	-2.523788	2.963672
Ag	0.388886	-0.041177	-3.466607
Ag	2.050941	-2.628828	0.160856

Au₂₀ (T_d)

Au	1.143764	-1.143764	1.143764
Au	1.143764	1.143764	-1.143764
Au	-1.143764	-1.143764	-1.143764
Au	-1.143764	1.143764	1.143764
Au	-0.965020	-0.965020	3.139895
Au	-0.965020	0.965020	-3.139895
Au	0.965020	-3.139895	-0.965020
Au	0.965020	3.139895	0.965020
Au	0.965020	-0.965020	-3.139895
Au	0.965020	0.965020	3.139895
Au	-0.965020	3.139895	-0.965020
Au	-0.965020	-3.139895	0.965020
Au	-3.139895	0.965020	-0.965020
Au	-3.139895	-0.965020	0.965020
Au	3.139895	0.965020	0.965020
Au	3.139895	-0.965020	-0.965020
Au	-2.936272	-2.936272	2.936272
Au	-2.936272	2.936272	-2.936272
Au	2.936272	-2.936272	-2.936272
Au	2.936272	2.936272	2.936272

Au₂₀ (C_s)

Au	-2.034344	-2.257472	0.000000
Au	-0.269331	2.280963	1.856217
Au	2.186303	-1.889419	-2.596775
Au	-0.720027	4.405194	0.000000
Au	-2.457470	1.995447	0.000000
Au	-2.164438	-0.043546	2.009111
Au	2.387359	0.828074	1.516032
Au	2.387359	0.828074	-1.516032
Au	-4.196584	-0.463294	0.000000
Au	-0.677323	-2.488496	-2.530198
Au	0.325543	0.052584	3.415163
Au	0.015154	-0.012593	0.000000
Au	-0.269331	2.280963	-1.856217
Au	0.727093	-2.802457	0.000000
Au	1.835879	3.164932	0.000000
Au	-0.677323	-2.488496	2.530198
Au	-2.164438	-0.043546	-2.009111
Au	2.186303	-1.889419	2.596775
Au	0.325543	0.052584	-3.415163
Au	3.254071	-1.510078	0.000000

Li₂₀ (*T_d*)

Li	1.085033	-1.085033	1.085033
Li	1.085033	1.085033	-1.085033
Li	-1.085033	-1.085033	-1.085033
Li	-1.085033	1.085033	1.085033
Li	-1.089298	-1.089298	3.199735
Li	-1.089298	1.089298	-3.199735
Li	1.089298	-3.199735	-1.089298
Li	1.089298	3.199735	1.089298
Li	1.089298	-1.089298	-3.199735
Li	1.089298	1.089298	3.199735
Li	-1.089298	3.199735	-1.089298
Li	-1.089298	-3.199735	1.089298
Li	-3.199735	1.089298	-1.089298
Li	-3.199735	-1.089298	1.089298
Li	3.199735	1.089298	1.089298
Li	3.199735	-1.089298	-1.089298
Li	-3.247494	-3.247494	3.247494
Li	-3.247494	3.247494	-3.247494
Li	3.247494	-3.247494	-3.247494
Li	3.247494	3.247494	3.247494

Li₂₀ (C_{2v})

Li	-1.675068	2.389219	-2.473481
Li	1.675068	2.389219	-2.473481
Li	1.675068	2.389219	2.473481
Li	-1.675068	2.389219	2.473481
Li	0.000000	-2.414929	2.327482
Li	0.000000	-2.414929	-2.327482
Li	-2.665938	-0.626066	-2.380857
Li	2.665938	-0.626066	-2.380857
Li	2.665938	-0.626066	2.380857
Li	-2.665938	-0.626066	2.380857
Li	2.553078	1.025944	0.000000
Li	-2.553078	1.025944	0.000000
Li	1.511467	-1.868062	0.000000
Li	-1.511467	-1.868062	0.000000
Li	0.000000	2.832068	0.000000
Li	0.000000	-4.473637	0.000000
Li	0.000000	0.212860	-3.977834
Li	0.000000	0.212860	3.977834
Li	0.000000	0.338665	-1.407951
Li	0.000000	0.338665	1.407951

Na₂₀ (*T_d*)

Na	1.344247	-1.344247	1.344247
Na	1.344247	1.344247	-1.344247
Na	-1.344247	-1.344247	-1.344247
Na	-1.344247	1.344247	1.344247
Na	-1.225530	-1.225530	3.901564
Na	-1.225530	1.225530	-3.901564
Na	1.225530	-3.901564	-1.225530
Na	1.225530	3.901564	1.225530
Na	1.225530	-1.225530	-3.901564
Na	1.225530	1.225530	3.901564
Na	-1.225530	3.901564	-1.225530
Na	-1.225530	-3.901564	1.225530
Na	-3.901564	1.225530	-1.225530
Na	-3.901564	-1.225530	1.225530
Na	3.901564	1.225530	1.225530
Na	3.901564	-1.225530	-1.225530
Na	-3.700098	-3.700098	3.700098
Na	-3.700098	3.700098	-3.700098
Na	3.700098	-3.700098	-3.700098
Na	3.700098	3.700098	3.700098

Na₂₀ (C_{2v})

Na	-1.984822	2.827626	-2.945697
Na	1.984822	2.827626	-2.945697
Na	1.984822	2.827626	2.945697
Na	-1.984822	2.827626	2.945697
Na	0.000000	-2.920085	2.701556
Na	0.000000	-2.920085	-2.701556
Na	-3.166878	-0.635777	-2.848816
Na	3.166878	-0.635777	-2.848816
Na	3.166878	-0.635777	2.848816
Na	-3.166878	-0.635777	2.848816
Na	3.409765	1.404550	0.000000
Na	-3.409765	1.404550	0.000000
Na	2.267063	-2.424209	0.000000
Na	-2.267063	-2.424209	0.000000
Na	0.000000	3.359079	0.000000
Na	0.000000	-5.249231	0.000000
Na	0.000000	0.266666	-4.737679
Na	0.000000	0.266666	4.737679
Na	0.000000	0.234457	-1.528485
Na	0.000000	0.234457	1.528485

Na₂₀ (C_s)

Na	-2.580083	-2.767175	0.000000
Na	-0.240161	2.698120	2.008383
Na	2.663207	-2.333401	-3.266462
Na	-0.892728	5.487071	0.000000
Na	-3.071383	2.414071	0.000000
Na	-2.644101	-0.105480	2.385419
Na	2.938873	1.113929	1.984476
Na	2.938873	1.113929	-1.984476
Na	-5.303966	-0.538531	0.000000
Na	-0.805808	-3.007260	-3.146901
Na	0.412011	0.072192	4.219582
Na	0.147138	-0.225335	0.000000
Na	-0.240161	2.698120	-2.008383
Na	0.883554	-3.578604	0.000000
Na	2.364720	4.070439	0.000000
Na	-0.805808	-3.007260	3.146901
Na	-2.644101	-0.105480	-2.385419
Na	2.663207	-2.333401	3.266462
Na	0.412011	0.072192	-4.219582
Na	3.804706	-1.738137	0.000000

$K_{20}(T_d)$

K	1.729246	-1.729246	1.729246
K	1.729246	1.729246	-1.729246
K	-1.729246	-1.729246	-1.729246
K	-1.729246	1.729246	1.729246
K	-1.581628	-1.581628	5.039806
K	-1.581628	1.581628	-5.039806
K	1.581628	-5.039806	-1.581628
K	1.581628	5.039806	1.581628
K	1.581628	-1.581628	-5.039806
K	1.581628	1.581628	5.039806
K	-1.581628	5.039806	-1.581628
K	-1.581628	-5.039806	1.581628
K	-5.039806	1.581628	-1.581628
K	-5.039806	-1.581628	1.581628
K	5.039806	1.581628	1.581628
K	5.039806	-1.581628	-1.581628
K	-4.781169	-4.781169	4.781169
K	-4.781169	4.781169	-4.781169
K	4.781169	-4.781169	-4.781169
K	4.781169	4.781169	4.781169

$\mathbf{K}_{20} (C_{2v})$

K	-2.515150	3.640141	-3.886864
K	2.515150	3.640141	-3.886864
K	2.515150	3.640141	3.886864
K	-2.515150	3.640141	3.886864
K	0.000000	-3.773706	3.530948
K	0.000000	-3.773706	-3.530948
K	-4.066357	-0.799430	-3.743096
K	4.066357	-0.799430	-3.743096
K	4.066357	-0.799430	3.743096
K	-4.066357	-0.799430	3.743096
K	4.328905	1.818709	0.000000
K	-4.328905	1.818709	0.000000
K	2.976405	-3.118917	0.000000
K	-2.976405	-3.118917	0.000000
K	0.000000	4.356626	0.000000
K	0.000000	-6.736652	0.000000
K	0.000000	0.294683	-6.190543
K	0.000000	0.294683	6.190543
K	0.000000	0.287820	-1.970548
K	0.000000	0.287820	1.970548

$K_{20}(C_8)$

K	-3.343154	-3.575608	0.000000
K	-0.322961	3.501299	2.643132
K	3.462197	-3.031114	-4.207854
K	-1.146265	7.097612	0.000000
K	-3.934140	3.101219	0.000000
K	-3.435973	-0.146421	3.132450
K	3.780515	1.438182	2.485263
K	3.780515	1.438182	-2.485263
K	-6.838239	-0.647318	0.000000
K	-1.018633	-3.902718	-4.046730
K	0.559242	0.074712	5.452375
K	0.116157	-0.252959	0.000000
K	-0.322961	3.501299	-2.643132
K	1.133734	-4.615467	0.000000
K	3.035777	5.307849	0.000000
K	-1.018633	-3.902718	4.046730
K	-3.435973	-0.146421	-3.132450
K	3.462197	-3.031114	4.207854
K	0.559242	0.074712	-5.452375
K	4.927355	-2.283207	0.000000

Rb₂₀ (T_d)

Rb	1.868370	-1.868370	1.868370
Rb	1.868370	1.868370	-1.868370
Rb	-1.868370	-1.868370	-1.868370
Rb	-1.868370	1.868370	1.868370
Rb	-1.680386	-1.680386	5.486450
Rb	-1.680386	1.680386	-5.486450
Rb	1.680386	-5.486450	-1.680386
Rb	1.680386	5.486450	1.680386
Rb	1.680386	-1.680386	-5.486450
Rb	1.680386	1.680386	5.486450
Rb	-1.680386	5.486450	-1.680386
Rb	-1.680386	-5.486450	1.680386
Rb	-5.486450	1.680386	-1.680386
Rb	-5.486450	-1.680386	1.680386
Rb	5.486450	1.680386	1.680386
Rb	5.486450	-1.680386	-1.680386
Rb	-5.085994	-5.085994	5.085994
Rb	-5.085994	5.085994	-5.085994
Rb	5.085994	-5.085994	-5.085994
Rb	5.085994	5.085994	5.085994

Rb₂₀ (C_{2v})

Rb	-2.710621	3.907292	-4.189014
Rb	2.710621	3.907292	-4.189014
Rb	2.710621	3.907292	4.189014
Rb	-2.710621	3.907292	4.189014
Rb	0.000000	-4.113124	3.834210
Rb	0.000000	-4.113124	-3.834210
Rb	-4.406074	-0.832212	-3.995224
Rb	4.406074	-0.832212	-3.995224
Rb	4.406074	-0.832212	3.995224
Rb	-4.406074	-0.832212	3.995224
Rb	4.769175	2.084506	0.000000
Rb	-4.769175	2.084506	0.000000
Rb	3.325990	-3.425330	0.000000
Rb	-3.325990	-3.425330	0.000000
Rb	0.000000	4.642260	0.000000
Rb	0.000000	-7.195008	0.000000
Rb	0.000000	0.366094	-6.673890
Rb	0.000000	0.366094	6.673890
Rb	0.000000	0.214068	-2.093662
Rb	0.000000	0.214068	2.093662

Rb₂₀ (C_s)

Rb	-3.607171	-3.846846	0.000000
Rb	-0.392936	3.756037	3.029701
Rb	3.761717	-3.283343	-4.529195
Rb	-1.195806	7.565798	0.000000
Rb	-4.163143	3.348630	0.000000
Rb	-3.732437	-0.170846	3.476794
Rb	4.044928	1.580211	2.661238
Rb	4.044928	1.580211	-2.661238
Rb	-7.294798	-0.637809	0.000000
Rb	-1.101643	-4.223444	-4.375621
Rb	0.652563	0.012867	5.941174
Rb	0.054252	-0.156778	0.000000
Rb	-0.392936	3.756037	-3.029701
Rb	1.189110	-4.866725	0.000000
Rb	3.238211	5.713749	0.000000
Rb	-1.101643	-4.223444	4.375621
Rb	-3.732437	-0.170846	-3.476794
Rb	3.761717	-3.283343	4.529195
Rb	0.652563	0.012867	-5.941174
Rb	5.314961	-2.462981	0.000000

Cs₂₀ (T_d)

Cs	2.067634	-2.067634	2.067634
Cs	2.067634	2.067634	-2.067634
Cs	-2.067634	-2.067634	-2.067634
Cs	-2.067634	2.067634	2.067634
Cs	-1.864896	-1.864896	6.109344
Cs	-1.864896	1.864896	-6.109344
Cs	1.864896	-6.109344	-1.864896
Cs	1.864896	6.109344	1.864896
Cs	1.864896	-1.864896	-6.109344
Cs	1.864896	1.864896	6.109344
Cs	-1.864896	6.109344	-1.864896
Cs	-1.864896	-6.109344	1.864896
Cs	-6.109344	1.864896	-1.864896
Cs	-6.109344	-1.864896	1.864896
Cs	6.109344	1.864896	1.864896
Cs	6.109344	-1.864896	-1.864896
Cs	-5.640405	-5.640405	5.640405
Cs	-5.640405	5.640405	-5.640405
Cs	5.640405	-5.640405	-5.640405
Cs	5.640405	5.640405	5.640405

Cs₂₀ (C_{2v})

Cs	-2.998968	4.336586	-4.674033
Cs	2.998968	4.336586	-4.674033
Cs	2.998968	4.336586	4.674033
Cs	-2.998968	4.336586	4.674033
Cs	0.000000	-4.574835	4.298102
Cs	0.000000	-4.574835	-4.298102
Cs	-4.882899	-0.928425	-4.466771
Cs	4.882899	-0.928425	-4.466771
Cs	4.882899	-0.928425	4.466771
Cs	-4.882899	-0.928425	4.466771
Cs	5.274729	2.316289	0.000000
Cs	-5.274729	2.316289	0.000000
Cs	3.700617	-3.779986	0.000000
Cs	-3.700617	-3.779986	0.000000
Cs	0.000000	5.155108	0.000000
Cs	0.000000	-7.949511	0.000000
Cs	0.000000	0.389701	-7.446508
Cs	0.000000	0.389701	7.446508
Cs	0.000000	0.229709	-2.327213
Cs	0.000000	0.229709	2.327213

Cs₂₀ (C_s)

Cs	3.038897	4.693558	-4.340763
Cs	-3.038897	4.693558	-4.340763
Cs	-2.932616	-4.720087	-4.311502
Cs	2.932616	-4.720087	-4.311502
Cs	0.000000	-4.365301	4.626276
Cs	0.000000	4.205157	4.576714
Cs	4.647242	4.580409	1.070179
Cs	-4.647242	4.580409	1.070179
Cs	-5.163407	-4.363715	0.789279
Cs	5.163407	-4.363715	0.789279
Cs	-5.217172	-0.015371	-2.342366
Cs	5.217172	-0.015371	-2.342366
Cs	-3.721635	-0.060535	3.769768
Cs	3.721635	-0.060535	3.769768
Cs	0.000000	-0.011016	-5.170605
Cs	0.000000	-0.081701	7.949547
Cs	0.000000	7.534068	-0.592130
Cs	0.000000	-7.429782	-0.203463
Cs	0.000000	2.300120	-0.303888
Cs	0.000000	-2.380065	-0.151640

Cs₂₀ (C_s)

Cs	-4.009561	-4.282969	0.000000
Cs	-0.454625	4.159176	3.395838
Cs	4.183013	-3.652293	-5.016373
Cs	-1.313498	8.402827	0.000000
Cs	-4.624114	3.748160	0.000000
Cs	-4.143865	-0.194064	3.867904
Cs	4.473343	1.748766	2.927517
Cs	4.473343	1.748766	-2.927517
Cs	-8.088974	-0.679777	0.000000
Cs	-1.220295	-4.699112	-4.858600
Cs	0.737660	0.004105	6.625850
Cs	0.023420	-0.157417	0.000000
Cs	-0.454625	4.159176	-3.395838
Cs	1.331766	-5.379223	0.000000
Cs	3.592095	6.358761	0.000000
Cs	-1.220295	-4.699112	4.858600
Cs	-4.143865	-0.194064	-3.867904
Cs	4.183013	-3.652293	5.016373
Cs	0.737660	0.004105	-6.625850
Cs	5.938404	-2.743518	0.000000

S-Figure 1. Schlegel diagram of a 20-vertex dodecahedron. Adding extra edges (dashed lines) in the pentagons lead to T_d symmetrical Au_{20} .