

Average Bond Length Differences by Model Chemistry

Calculated at QCISD(T)/6-311G*

Species	Name	Bond type	Bond Length (Å)					
			Experimental	unc.	Calculated	Difference	atom1	atom2
LiO	lithium oxide	rLiO	1.688		1.593	-0.096	1	2
CuF	Copper monofluoride	rCuF	1.745	±0.000	1.721	-0.024	1	2
LiOH	lithium hydroxide	rOH	0.969		0.951	-0.018	1	3
CuH	Copper monohydride	rCuH	1.463		1.448	-0.015	1	2
LiOH	lithium hydroxide	rLiO	1.582		1.575	-0.006	1	2
FNO ₂	Nitryl fluoride	rNF	1.467	±0.015	1.462	-0.005	1	2
SiH ₂ Cl ₂	dichlorosilane	rSiH	1.480	±0.015	1.475	-0.005	1	2
NH ₄ ⁺	ammonium cation	rHN	1.029	±0.000	1.024	-0.005	1	2
CH ₂ NH	Methanimine	rCH	1.103		1.100	-0.003	1	3
CH ₃ NH ₂	methyl amine	rNH	1.018	±0.001	1.016	-0.002	2	6
CH ₂	Methylene	rCH	1.085		1.084	-0.001	1	2
CH ₂ PH	H2CPH	rCH	1.090	±0.015	1.089	-0.001	1	3
CH ₃ NH ₂	methyl amine	rCN	1.471	±0.003	1.471	0.000	1	2
CH ₂ PH	H2CPH	rCH	1.090	±0.015	1.090	0.000	1	4
HS ⁺	sulfur monohydride cation	rSH	1.374		1.375	0.000	1	2
DF	Hydrofluoric acid-d	rDF	0.917	±0.000	0.918	0.001	1	2
H ₂ O	Water	rOH	0.958	±0.000	0.959	0.001	1	2
HO ₂	Hydroperoxy radical	rOH	0.971		0.972	0.001	1	3
HF	Hydrogen fluoride	rHF	0.917	±0.000	0.918	0.001	1	2
LiCl	lithium chloride	rLiCl	2.021	±0.000	2.023	0.002	1	2
HO ₂	Hydroperoxy radical	rOO	1.331		1.333	0.002	1	2
DO	Hydroxyl-d	rDO	0.970		0.973	0.003	1	2
OH	Hydroxyl radical	rOH	0.970		0.973	0.003	1	2
O ₂	Oxygen diatomic	rO=O	1.208		1.211	0.004	1	2
C ₂ H ₂ ClF	1-chloro-1-fluoroethylene	rCH	1.082	±0.001	1.086	0.004	2	5
C ₂ H	Ethynyl radical	rC#C	1.217		1.221	0.004	1	2
D ₂	Deuterium diatomic	rDD	0.742		0.746	0.005	1	2
H ₂	Hydrogen diatomic	rHH	0.741		0.746	0.005	1	2
HD	Deuterium hydride	rDH	0.741		0.746	0.005	1	2
C ₄ H ₈	cyclobutane	rCH	1.093		1.099	0.005	1	5

C ₃ H ₆	Cyclopropane	rCH	1.083		1.088	0.005	1	4
C ₂ H ₂	Acetylene	rCH	1.063		1.069	0.006	1	3
LiF	lithium fluoride	rLiF	1.564	±0.000	1.570	0.006	1	2
NF	nitrogen fluoride	rNF	1.317		1.323	0.006	1	2
BCl	boron monochloride	rBCl	1.719	±0.000	1.726	0.006	1	2
CH ₃ I	methyl iodide	rCH	1.084	±0.003	1.090	0.006	1	3
BeO	beryllium oxide	rBe=O	1.331		1.337	0.006	1	2
C ₄ H ₈	cyclobutane	rCH	1.091		1.097	0.006	1	6
SiH ₃ Cl	chlorosilane	rSiH	1.475		1.482	0.007	1	3
SiH ₃ F	monofluorosilane	rSiH	1.476		1.483	0.007	1	3
FNO ₂	Nitryl fluoride	rN=O	1.180	±0.005	1.187	0.007	1	3
NH	Imidogen	rNH	1.036		1.043	0.007	1	2
CH ₄	Methane	rCH	1.087	±0.001	1.094	0.007	1	2
NO ⁺	nitric oxide cation	rN=O	1.066		1.073	0.007	1	2
TiCl	Titanium Monochloride	rClTi	2.265	±0.000	2.272	0.007	1	2
BF	Boron monofluoride	rBF	1.267	±0.000	1.274	0.007	1	2
NO	Nitric oxide	rN=O	1.154	±0.000	1.162	0.008	1	2
SiH ₄	Silane	rSiH	1.480	±0.000	1.488	0.008	1	2
BeCl	beryllium monochloride	rBeCl	1.797		1.805	0.008	1	2
SiN	Silicon nitride	rSiN	1.575		1.584	0.009	1	2
BF ₃	Borane, trifluoro-	rBF	1.307		1.316	0.009	1	2
SOCl ₂	thionyl chloride	rS=O	1.443	±0.006	1.452	0.009	1	2
CO	Carbon monoxide	rC#O	1.128	±0.000	1.138	0.009	1	2
BO	boron monoxide	rB=O	1.205		1.214	0.009	1	2
BH ₃	boron trihydride	rBH	1.190		1.200	0.010	1	2
HCl ⁺	hydrogen chloride cation	rHCl	1.315		1.324	0.010	1	2
P ₂ H ₄	H2PPH2	rPH	1.417		1.427	0.010	1	3
N ₃	azide radical	rNN	1.181		1.191	0.010	1	2
SiH ⁺	silicon monohydride cation	rSiH	1.504		1.515	0.010	1	2
CH	Methylidyne	rCH	1.120		1.130	0.010	1	2
CP	Carbon monophosphide	rC#P	1.562		1.573	0.011	1	2
MgOH	magnesium hydroxide	rOH	0.940		0.951	0.011	1	3
P ₂ H ₄	H2PPH2	rPH	1.414		1.425	0.011	1	4
FO	Oxygen monofluoride	rFO	1.354		1.365	0.011	1	2
CH ₃ NH ₂	methyl amine	rCH	1.093	±0.000	1.104	0.011	1	3
C ₂ H ₃	vinyl	rCH	1.085		1.097	0.012	2	4
N ₂	Nitrogen diatomic	rN#N	1.098		1.110	0.012	1	2
SiH ₃ ⁺	Silyl cation	rSiH	1.460	±0.010	1.472	0.012	1	2
CN	Cyano radical	rC#N	1.172		1.184	0.012	1	2

C ₂ H ₂	Acetylene	rC#C	1.203		1.216	0.013	1	2
C ₃ H ₆	Cyclopropane	rCC	1.501		1.515	0.014	1	2
OH ⁻	hydroxide anion	rOH	0.964		0.978	0.014	1	2
BeH ₂	beryllium dihydride	rBeH	1.326	±0.000	1.341	0.015	1	2
PN	Phosphorus mononitride	rP#N	1.491		1.506	0.015	1	2
H ₂ CS	Thioformaldehyde	rC=S	1.611		1.626	0.015	1	2
BH	Boron monohydride	rBH	1.232		1.248	0.015	1	2
AlH	aluminum monohydride	rAlH	1.648		1.663	0.015	1	2
AlC	Aluminum carbide	rC=Al	1.955		1.971	0.015	1	2
SiH ₃ Cl	chlorosilane	rSiCl	2.051		2.067	0.016	1	2
SiH ₂ Cl ₂	dichlorosilane	rSiCl	2.033	±0.003	2.049	0.016	1	4
LiBr	Lithium Bromide	rLiBr	2.170	±0.000	2.187	0.016	1	2
C ₁₀ H ₈	naphthalene	rC:C	1.410		1.427	0.017	2	3
BeF	Beryllium monofluoride	rBeF	1.361		1.378	0.017	1	2
DCl	Hydrochloric acid-d	rDCl	1.275	±0.000	1.292	0.017	1	2
HCl	Hydrogen chloride	rHCl	1.275	±0.000	1.292	0.017	1	2
HS	Mercapto radical	rSH	1.341		1.358	0.017	1	2
PH	phosphorus monohydride	rPH	1.422		1.440	0.017	1	2
DS	Mercapto-d	rSD	1.341		1.358	0.018	1	2
CaF	Calcium monofluoride	rFCa	1.967	±0.001	1.985	0.018	1	2
C ₄ H ₆	Bicyclo[1.1.0]butane	rCC	1.497		1.515	0.018	1	2
CS	carbon monosulfide	rC#S	1.535		1.553	0.018	1	2
SiH	Silylidyne	rSiH	1.520		1.538	0.018	1	2
SiO	Silicon monoxide	rSiO	1.510	±0.000	1.528	0.018	1	2
BS	boron sulfide	rBS	1.609		1.628	0.018	1	2
PS	phosphorus sulfide	rP=S	1.900		1.919	0.019	1	2
C ₂	Carbon diatomic	rC=C	1.243		1.261	0.019	1	2
AlS	Aluminum sulfide	rAlS	2.029		2.048	0.019	1	2
Li ₂	Lithium diatomic	rLiLi	2.673		2.693	0.020	1	2
NaF	sodium fluoride	rNaF	1.926	±0.000	1.946	0.020	1	2
BeH	beryllium monohydride	rBeH	1.343		1.363	0.020	1	2
SiS	silicon monosulfide	rSiS	1.929	±0.000	1.950	0.020	1	2
P ₂	Phosphorus diatomic	rP#P	1.893		1.914	0.020	1	2
NS	Mononitrogen monosulfide	rNS	1.497	±0.000	1.518	0.021	1	2
CaOH	Calcium monohydroxide	rOCa	1.976	±0.004	1.998	0.022	1	2
SiH ₃ F	monofluorosilane	rSiF	1.595		1.616	0.022	1	2
SiCl	Clorosilylidyne	rSiCl	2.061	±0.000	2.083	0.022	1	2
BeS	beryllium sulfide	rBe=S	1.742		1.764	0.022	1	2
CaOH	Calcium monohydroxide	rOH	0.930	±0.007	0.952	0.022	2	3
LiH	Lithium Hydride	rLiH	1.595	±0.000	1.618	0.023	1	2

PO	Phosphorus monoxide	rP=O	1.476		1.499	0.023	1	2
SiF	silicon monofluoride	rSiF	1.604		1.627	0.023	1	2
C ₂ H	Ethynyl radical	rCH	1.047		1.070	0.023	1	3
HS ⁻	mercapto anion	rSH	1.343		1.366	0.023	1	2
C ₃ H ₅	Allyl radical	rCH	1.069		1.093	0.024	1	2
CSe	Carbon monoselenide	rC=Se	1.676	±0.000	1.702	0.025	1	2
Si ₂	Silicon diatomic	rSiSi	2.246		2.272	0.026	1	2
NSe	Nitrogen monoselenide	rN=Se	1.652		1.678	0.026	1	2
MgOH	magnesium hydroxide	rMgO	1.767		1.793	0.026	1	2
NaCl	Sodium Chloride	rNaCl	2.361	±0.000	2.387	0.026	1	2
AlF	Aluminum monofluoride	rAlF	1.654	±0.000	1.681	0.027	1	2
MgCl	magnesium monochloride	rMgCl	2.199		2.227	0.028	1	2
CuCl	Copper monochloride	rCuCl	2.051	±0.000	2.079	0.028	1	2
CCl	carbon monochloride	rCCl	1.649		1.678	0.029	1	2
H ₂ Se	Hydrogen selenide	rSeH	1.460		1.489	0.029	1	2
PF	phosphorus monofluoride	rFP	1.593		1.623	0.030	1	2
SO	Sulfur monoxide	rS=O	1.481		1.512	0.031	1	2
MgF	Magnesium monofluoride	rMgF	1.750		1.782	0.032	1	2
CH ₃ I	methyl iodide	rCI	2.136	±0.002	2.168	0.033	1	2
SOF ₄	Sulfur tetrafluoride oxide	rFS	1.596	±0.003	1.629	0.033	1	3
NaBr	Sodium Bromide	rNaBr	2.502	±0.000	2.536	0.034	1	2
GeH	germylidene	rGeH	1.588		1.623	0.035	1	2
S ₂	Sulfur diatomic	rS=S	1.889		1.926	0.037	1	2
MgS	magnesium sulfide	rMgS	2.143		2.179	0.037	1	2
MgH	magnesium monohydride	rMgH	1.730		1.768	0.038	1	2
SF	Monosulfur monofluoride	rSF	1.599		1.639	0.040	1	2
ClO	Monochlorine monoxide	rClO	1.596	±0.001	1.636	0.040	1	2
SOF ₄	Sulfur tetrafluoride oxide	rFS	1.539	±0.003	1.580	0.041	1	5
HI	Hydrogen iodide	rHI	1.609	±0.000	1.651	0.042	1	2
NaH	sodium hydride	rNaH	1.887	±0.000	1.929	0.042	1	2
PCl	phosphorus chloride	rPCl	2.018		2.060	0.043	1	2
MgO	magnesium oxide	rMgO	1.749		1.795	0.046	1	2
CFCl	chlorofluoromethylene	rCCl	1.714		1.761	0.047	1	3
HOCl	hypochlorous acid	rClO	1.691		1.738	0.047	1	3
CaCl	calcium monochloride	rClCa	2.437		2.484	0.048	1	2
KH	Potassium hydride	rKH	2.243	±0.001	2.291	0.048	1	2
NaLi	lithium sodium	rLiNa	2.889		2.941	0.052	1	2

GeF ⁺	Germanium monofluoride cation	rFGe	1.665	±0.000	1.720	0.054	1	2
He ₂ ⁺	helium dimer cation	rHeHe	1.081	±0.001	1.138	0.057	1	2
CaH	Calcium monohydride	rCaH	2.003	±0.000	2.061	0.058	1	2
SCl	sulfur monochloride	rSCl	1.975		2.035	0.060	1	2
IBr	Iodine monobromide	rBrI	2.469	±0.000	2.531	0.062	1	2
Cl ₂	Chlorine diatomic	rClCl	1.988		2.052	0.064	1	2
ClOF ₃	Chlorine trifluoride oxide	rFCl	1.713	±0.003	1.779	0.066	1	4
IF	Iodine monofluoride	rFI	1.910		1.978	0.069	1	2
ICl	Iodine monochloride	rClI	2.321	±0.000	2.392	0.071	1	2
I ₂	Iodine diatomic	rII	2.665		2.744	0.078	1	2
ClOF ₃	Chlorine trifluoride oxide	rFCl	1.603	±0.004	1.711	0.108	1	3