

Supporting Information for:

Experimental and Theoretical Studies of the Infrared Spectra and Bonding

Properties of NgBeCO_3 and a Comparison with NgBeO ($\text{Ng} = \text{He, Ne, Ar, Kr, Xe}$)

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Full references 56 and 57.

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Table S1. Coordinates and energies of the calculated molecules.

Cartesian coordinates of the optimized structure.

CO

BeO

E(M06-2X/def2-TZVPP) = -89.8963962

Be	0.000000000000	0.000000000000	-0.878688000000
O	0.000000000000	0.000000000000	0.439344000000

BeO

E(MP2/cc-pVTZ) = -89.742503153430

Be	0.000000000000	0.000000000000	-0.8964929222
O	0.000000000000	0.000000000000	0.4571489222

BeO

E(CCSD(T)/cc-pVTZ) = -89.748243856625

Be	0.0000000000	0.0000000000	-0.8919102512
O	0.0000000000	0.0000000000	0.4525662512

BeCO₃

E(M06-2X/def2-TZVPP) = -278.5956542

Be	1.485898000000	0.000038000000	-0.000001000000
O	0.510242000000	1.096671000000	0.000000000000
C	-0.333926000000	0.000040000000	0.000002000000
O	0.510401000000	-1.096631000000	0.000000000000
O	-1.513148000000	-0.000089000000	-0.000001000000

BeCO₃

E(MP2/cc-pVTZ) = -278.135187293601

Be	1.489208401400	0.000065119800	-0.000001009400
O	0.514608725100	1.111634332300	0.000000202700
C	-0.335431496900	-0.000002880100	0.000001337000
O	0.514731314900	-1.111587868400	0.000000202800
O	-1.523649944600	-0.000079703600	-0.000000733100

BeCO₃

E(CCSD(T)/cc-pVTZ) = -278.16643051

Be	1.4894426960	0.0000670497	-0.0000010675
O	0.5152668743	1.1082859630	0.0000002414
C	-0.3364820020	-0.0000052123	0.0000013489
O	0.5153865048	-1.1082396870	0.0000002415
O	-1.5241470731	-0.0000791136	-0.0000007642

He-BeO

E(M06-2X/def2-TZVPP) = -92.8083279

He	0.000000000000	0.000000000000	-2.053572000000
Be	0.000000000000	0.000000000000	-0.534491000000
O	0.000000000000	0.000000000000	0.780638000000

He-BeO

E(MP2/cc-pVTZ) = -92.644999259873

He	0.000000000000	0.000000000000	-2.064708132100
Be	0.000000000000	0.000000000000	-0.544179555700
O	0.000000000000	0.000000000000	0.801462687900

He-BeO

E(CCSD(T)/cc-pVTZ) = -92.656231137751

He	0.000000000000	0.000000000000	-2.062685741300
Be	0.000000000000	0.000000000000	-0.540284882600

O	0.000000000000	0.000000000000	0.795545624000
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He-BeCO₃

E(M06-2X/def2-TZVPP) = -281.5039435

He	2.932098000000	-0.002944000000	-0.005987000000
Be	1.323365000000	0.002196000000	0.001928000000
O	0.337961000000	-1.091919000000	0.000978000000
C	-0.507546000000	-0.000497000000	0.000083000000
O	0.335360000000	1.093586000000	0.000968000000
O	-1.687369000000	-0.001657000000	-0.001475000000

He-BeCO₃

E(MP2/cc-pVTZ) = -281.034628272551

He	2.9384218586	-0.0000205458	-0.0034160606
Be	1.3271921305	-0.0000687409	-0.0005943350
O	0.3396768948	-1.1062179801	-0.0001140122
C	-0.5110339343	-0.0003460616	0.0002392888
O	0.3394914748	1.1058243749	-0.0001410811
O	-1.6998794244	-0.0004060465	0.0005212001

He-BeCO₃

E(CCSD(T)/cc-pVTZ) = -281.072152376714

He	2.9346272799	-0.0000125503	-0.0034379228
Be	1.3281993893	-0.0000759574	-0.0005632308
O	0.3410901573	-1.1029288966	-0.0001037081
C	-0.5113176226	-0.0003421210	0.0002350665
O	0.3409089774	1.1025281648	-0.0001305113
O	-1.6996391813	-0.0004036395	0.0004953065

Ne-BeO

E(M06-2X/def2-TZVPP) = -218.837999

Ne	0.000000000000	0.000000000000	1.457398000000
Be	0.000000000000	0.000000000000	-0.336788000000
O	0.000000000000	0.000000000000	-1.653353000000

Ne-BeO

E(MP2/cc-pVTZ) = -218.548418594182

Ne	0.000000000000	0.000000000000	1.468497242100
Be	0.000000000000	0.000000000000	-0.327155495600
O	0.000000000000	0.000000000000	-1.674084746400

Ne-BeO

E(CCSD(T)/cc-pVTZ) = -218.560316060725

Ne	0.000000000000	0.000000000000	1.460709461100
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Be	0.000000000000	0.000000000000	-0.328096150100
O	0.000000000000	0.000000000000	-1.665356311000

Ne-BeCO₃

E(M06-2X/def2-TZVPP) = -407.5355902

Ne	0.000000000000	0.000000000000	2.580192000000
Be	0.000000000000	0.000000000000	0.738384000000
O	0.000000000000	1.092866000000	-0.250389000000
C	0.000000000000	0.000000000000	-1.093240000000
O	0.000000000000	-1.092866000000	-0.250389000000
O	0.000000000000	0.000000000000	-2.273725000000

Ne-BeCO₃

E(MP2/cc-pVTZ) = -406.940730672422

Ne	0.000000000000	0.000000000000	2.560688488500
Be	0.000000000000	0.000000000000	0.747641327500
O	0.000000000000	1.105605055100	-0.242276952800
C	0.000000000000	0.000000000000	-1.091739473700
O	0.000000000000	-1.105605055100	-0.242276952800
O	0.000000000000	0.000000000000	-2.281203436600

Ne-BeCO₃

E(CCSD(T)/cc-pVTZ) = -406.978709593099

Ne	0.000000000000	0.000000000000	2.549403765200
Be	0.000000000000	0.000000000000	0.750082758100
O	0.000000000000	1.102249881700	-0.239288889400
C	0.000000000000	0.000000000000	-1.090592511000
O	0.000000000000	-1.102249881700	-0.239288889400
O	0.000000000000	0.000000000000	-2.279483233400

Ar-BeO

E(M06-2X/def2-TZVPP) = -617.4403015

Ar	0.000000000000	0.000000000000	1.179418000000
Be	0.000000000000	0.000000000000	-0.890005000000
O	0.000000000000	0.000000000000	-2.208687000000

Ar-BeO

E(MP2/cc-pVTZ) = -616.780538456923

Ar	0.000000000000	0.000000000000	1.6554384298
Be	0.000000000000	0.000000000000	-0.4205124197
O	0.000000000000	0.000000000000	-1.7676690101

Ar-BeO

E(CCSD(T)/cc-pVTZ) = -616.810661029563

Ar	0.0000000000	0.0000000000	1.6491334923
Be	0.0000000000	0.0000000000	-0.4218349969
O	0.0000000000	0.0000000000	-1.7600414954

Ar-BeCO₃

E(M06-2X/def2-TZVPP) = -806.1360107

Ar	0.000000000000	0.000000000000	2.366224000000
Be	0.000000000000	0.000000000000	0.255962000000
O	0.000000000000	1.089829000000	-0.746247000000
C	0.000000000000	0.000000000000	-1.587082000000
O	0.000000000000	-1.089829000000	-0.746247000000
O	0.000000000000	0.000000000000	-2.769178000000

Ar-BeCO₃

E(MP2/cc-pVTZ) = -805.171060839501

Ar	0.000000000000	0.000000000000	2.817281932900
Be	0.000000000000	0.000000000000	0.706041798700
O	0.000000000000	1.102800399900	-0.296874027700
C	0.000000000000	0.000000000000	-1.143877386700
O	0.000000000000	-1.102800399900	-0.296874027700
O	0.000000000000	0.000000000000	-2.334865289500

Ar-BeCO₃

E(CCSD(T)/cc-pVTZ) = -805.226928321526

Ar	0.000000000000	0.000000000000	2.814577982600
Be	0.000000000000	0.000000000000	0.707197758600
O	0.000000000000	1.099511675000	-0.295805841600
C	0.000000000000	0.000000000000	-1.144411108700
O	0.000000000000	-1.099511675000	-0.295805841600
O	0.000000000000	0.000000000000	-2.334919949300

Kr-BeO

E(M06-2X/def2-TZVPP) = -2843.7362211

Kr	0.000000000000	0.000000000000	0.775229000000
Be	0.000000000000	0.000000000000	-1.445749000000
O	0.000000000000	0.000000000000	-2.765658000000

Kr-BeO

E(MP2/cc-pVTZ) = -2841.988639588787

Kr	0.000000000000	0.000000000000	0.778941400600
Be	0.000000000000	0.000000000000	-1.433522254300
O	0.000000000000	0.000000000000	-2.781597146300

Kr-BeO

E(CCSD(T)/cc-pVTZ) = -2842.015994953367

Kr	0.000000000000	0.000000000000	0.773487753700
Be	0.000000000000	0.000000000000	-1.435203654600
O	0.000000000000	0.000000000000	-2.774462099000

Kr-BeCO₃

E(M06-2X/def2-TZVPP) = -3032.431313

Kr	0.000000000000	0.000000000000	1.837138000000
Be	0.000000000000	0.000000000000	-0.431627000000
O	0.000000000000	1.088970000000	-1.439849000000
C	0.000000000000	0.000000000000	-2.279299000000
O	0.000000000000	-1.088970000000	-1.439849000000
O	0.000000000000	0.000000000000	-3.462133000000

Kr-BeCO₃

E(MP2/cc-pVTZ) = -3030.378180580075

Kr	0.000000000000	0.000000000000	1.832431797300
Be	0.000000000000	0.000000000000	-0.427186887000
O	0.000000000000	1.102303491000	-1.434207581800
C	0.000000000000	0.000000000000	-2.280553960900
O	0.000000000000	-1.102303491000	-1.434207581800
O	0.000000000000	0.000000000000	-3.471894785900

Kr-BeCO₃

E(CCSD(T)/cc-pVTZ) = -3030.431188888698

Kr	0.000000000000	0.000000000000	1.828880416100
Be	0.000000000000	0.000000000000	-0.425765538500
O	0.000000000000	1.098887639300	-1.433093583100
C	0.000000000000	0.000000000000	-2.280764170000
O	0.000000000000	-1.098887639300	-1.433093583100
O	0.000000000000	0.000000000000	-3.471782541400

Xe-BeO

E(M06-2X/def2-TZVPP) = -419.2187276

Xe	0.000000000000	0.000000000000	0.597916000000
Be	0.000000000000	0.000000000000	-1.809800000000
O	0.000000000000	0.000000000000	-3.131033000000

Xe-BeO

E(MP2/cc-pVTZ&cc-pVTZ-PP) = -418.213460086664

Xe	0.000000000000	0.000000000000	0.594886570900
Be	0.000000000000	0.000000000000	-1.794251069000

O	0.000000000000	0.000000000000	-3.143552501900
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Xe-BeO

E(CCSD(T)/cc-pVTZ&cc-pVTZ-PP) = -418.239798822025

Xe	0.000000000000	0.000000000000	0.589331007700
Be	0.000000000000	0.000000000000	-1.795822927100
O	0.000000000000	0.000000000000	-3.136425080600

Xe-BeCO₃

E(M06-2X/def2-TZVPP) = -607.913112

Xe	0.000000000000	0.000000000000	1.535852000000
Be	0.000000000000	0.000000000000	-0.923092000000
O	0.000000000000	1.088508000000	-1.934584000000
C	0.000000000000	0.000000000000	-2.773055000000
O	0.000000000000	-1.088508000000	-1.934584000000
O	0.000000000000	0.000000000000	-3.956493000000

Xe-BeCO₃

E(MP2/cc-pVTZ&cc-pVTZ-PP) = -606.601760992366

Xe	0.000000000000	0.000000000000	1.528184627500
Be	0.000000000000	0.000000000000	-0.916905357500
O	0.000000000000	1.101554973600	-1.928867319000
C	0.000000000000	0.000000000000	-2.773667519600
O	0.000000000000	-1.101554973600	-1.928867319000
O	0.000000000000	0.000000000000	-3.965833112400

Xe-BeCO₃

E(CCSD(T)/cc-pVTZ&cc-pVTZ-PP) = -606.653625281976

Xe	0.000000000000	0.000000000000	1.526992849900
Be	0.000000000000	0.000000000000	-0.915720216500
O	0.000000000000	1.098211810800	-1.928224305300
C	0.000000000000	0.000000000000	-2.774522990800
O	0.000000000000	-1.098211810800	-1.928224305300
O	0.000000000000	0.000000000000	-3.966257032000