

Accessory Publication

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Matrix Isolation and Electronic Structure of Di- and Tridehydrobenzenes**1** (1A_1): BLYP/cc-pVTZ, E = -230.905574

C	0.000000	1.464639	-0.135200
C	0.000000	0.703974	1.062606
C	0.000000	0.626551	-1.240499
C	0.000000	-0.703974	1.062606
C	0.000000	-0.626551	-1.240499
C	0.000000	-1.464639	-0.135200
H	0.000000	2.550883	-0.136000
H	0.000000	1.233794	2.014564
H	0.000000	-1.233794	2.014564
H	0.000000	-2.550883	-0.136000

1 (1A_1): CCSD(T)/cc-pVTZ, E = -230.47777830, T1: 0.01295

C	0.000000	1.461977	-0.129287
C	0.000000	-1.461977	-0.129287
C	0.000000	0.705293	1.059714
C	0.000000	-0.705293	1.059714
C	0.000000	0.630153	-1.243649
C	0.000000	-0.630153	-1.243649
H	0.000000	2.542813	-0.130951
H	0.000000	-2.542813	-0.130951
H	0.000000	1.226413	2.010290
H	0.000000	-1.226413	2.010290

1 (1A_1): CCSD(T)/cc-pVQZ, E = -230.54230169, T1: 0.01321

C	0.0000000000	1.4591594832	-0.1289781396
C	0.0000000000	-1.4591594832	-0.1289781396
C	0.0000000000	0.7040162609	1.0577788915
C	0.0000000000	-0.7040162609	1.0577788915
C	0.0000000000	0.6283097127	-1.2405234391
C	0.0000000000	-0.6283097127	-1.2405234391
H	0.0000000000	2.5394910205	-0.1298405316
H	0.0000000000	-2.5394910205	-0.1298405316
H	0.0000000000	1.2252217910	2.0076802187
H	0.0000000000	-1.2252217910	2.0076802187

1 (1A_1): RS2/cc-pVTZ, E = -230.41421576

C	0.0000000000	1.4575049092	-0.1306249787
C	0.0000000000	-1.4575049092	-0.1306249787
C	0.0000000000	0.7018517530	1.0619450026
C	0.0000000000	-0.7018517530	1.0619450026

S2

C	0.0000000000	0.6336591904	-1.2437473766
C	0.0000000000	-0.6336591904	-1.2437473766
H	0.0000000000	2.5362276950	-0.1302349136
H	0.0000000000	-2.5362276950	-0.1302349136
H	0.0000000000	1.2247624722	2.0087792664
H	0.0000000000	-1.2247624722	2.0087792664

1(³B₂): UBLYP/cc-pVTZ, E = -230.8480337, S2 = 2.0061

C	0.000000	1.409852	-0.118132
C	0.000000	0.698778	1.101140
C	0.000000	0.700613	-1.302712
C	0.000000	-0.698778	1.101140
C	0.000000	-0.700613	-1.302712
C	0.000000	-1.409852	-0.118132
H	0.000000	2.500756	-0.123094
H	0.000000	1.247323	2.041315
H	0.000000	-1.247323	2.041315
H	0.000000	-2.500756	-0.123094

1(³B₂): RCCSD(T)/cc-pVTZ, E = -230.41874248, T1: 0.01496

C	0.0000000000	1.4114473226	-0.1214081807
C	0.0000000000	0.6974632036	1.0913917741
C	0.0000000000	0.7007852515	-1.3067617728
C	0.0000000000	-0.6974632036	1.0913917741
C	0.0000000000	-0.7007852515	-1.3067617728
C	0.0000000000	-1.4114473226	-0.1214081807
H	0.0000000000	2.4952231815	-0.1265039025
H	0.0000000000	1.2400060532	2.0287530819
H	0.0000000000	-1.2400060532	2.0287530819
H	0.0000000000	-2.4952231815	-0.1265039025

1(³B₂): RS2/cc-pVTZ, E = -230.35874542

C	0.0000000000	1.4111020940	-0.1195781674
C	0.0000000000	0.6975546283	1.0900028604
C	0.0000000000	0.7001733355	-1.3052830646
C	0.0000000000	-0.6975546283	1.0900028604
C	0.0000000000	-0.7001733355	-1.3052830646
C	0.0000000000	-1.4111020940	-0.1195781674
H	0.0000000000	2.4925389255	-0.1254001277
H	0.0000000000	1.2382095100	2.0257294992
H	0.0000000000	-1.2382095100	2.0257294992
H	0.0000000000	-2.4925389255	-0.1254001277

2(¹A₁): BLYP/cc-pVTZ, E = -230.8859627

C	0.000000	0.000000	1.643580
C	0.000000	0.998616	0.710835
C	0.000000	1.174413	-0.651908
C	0.000000	0.000000	-1.430232
C	0.000000	-1.174413	-0.651908
C	0.000000	-0.998616	0.710835
H	0.000000	0.000000	2.728318
H	0.000000	2.167364	-1.096451
H	0.000000	0.000000	-2.522623
H	0.000000	-2.167364	-1.096451

2(¹A₁): CCSD(T)/cc-pVTZ, E = -230.45653797, T1: 0.01570

C	0.000000	0.000000	1.624697
C	0.000000	1.028970	0.717612
C	0.000000	-1.028970	0.717612
C	0.000000	1.175385	-0.653053
C	0.000000	-1.175385	-0.653053
C	0.000000	0.000000	-1.419340

S3

H	0.000000	0.000000	2.702158
H	0.000000	2.160055	-1.101738
H	0.000000	-2.160055	-1.101738
H	0.000000	0.000000	-2.505539

2(¹A₁): CCSD(T)/cc-pVQZ, E = -230.52050120, T1: 0.015683

C	0.0000000000	0.0000000000	1.6252791257
C	0.0000000000	1.0198369572	0.7140523126
C	0.0000000000	-1.0198369572	0.7140523126
C	0.0000000000	1.1722676994	-0.6528667604
C	0.0000000000	-1.1722676994	-0.6528667604
C	0.0000000000	0.0000000000	-1.4192327872
H	0.0000000000	0.0000000000	2.7024778352
H	0.0000000000	2.1575767635	-1.0992040976
H	0.0000000000	-2.1575767635	-1.0992040976
H	0.0000000000	0.0000000000	-2.5048690828

2(¹A₁): RS2/cc-pVTZ, E = -230.39673535

C	0.0000000000	0.0000000000	1.6086429004
C	0.0000000000	1.0518485420	0.7225348705
C	0.0000000000	-1.0518485420	0.7225348705
C	0.0000000000	1.1778889718	-0.6482049563
C	0.0000000000	-1.1778889718	-0.6482049563
C	0.0000000000	0.0000000000	-1.4083321180
H	0.0000000000	0.0000000000	2.6838910833
H	0.0000000000	2.1559358757	-1.1066431066
H	0.0000000000	-2.1559358757	-1.1066431066
H	0.0000000000	0.0000000000	-2.4919574809

2(³B₂): UBLYP/cc-pVTZ, E = -230.8545876, S2 = 2.01249

C	0.000000	0.000000	1.485537
C	0.000000	1.170145	0.742528
C	0.000000	1.230585	-0.637933
C	0.000000	0.000000	-1.326588
C	0.000000	-1.230585	-0.637933
C	0.000000	-1.170145	0.742528
H	0.000000	0.000000	2.576269
H	0.000000	2.171112	-1.184186
H	0.000000	0.000000	-2.416729
H	0.000000	-2.171112	-1.184186

2(³B₂): RCCSD(T)/cc-pVTZ, E = -230.42442168, T1: 0.015359

C	0.0000000000	0.0000000000	1.4858338504
C	0.0000000000	1.1702244637	0.7419681456
C	0.0000000000	1.2262361386	-0.6399512853
C	0.0000000000	0.0000000000	-1.3271345986
C	0.0000000000	-1.2262361386	-0.6399512853
C	0.0000000000	-1.1702244637	0.7419681456
H	0.0000000000	0.0000000000	2.5691752158
H	0.0000000000	2.1631043637	-1.1807311114
H	0.0000000000	0.0000000000	-2.4111389654
H	0.0000000000	-2.1631043637	-1.1807311114

2(³B₂): RS2/cc-pVTZ, E = -230.36474043

C	0.0000000000	0.0000000000	1.4847985586
C	0.0000000000	1.1683582566	0.7406955401
C	0.0000000000	1.2254017980	-0.6397496951
C	0.0000000000	0.0000000000	-1.3260004739
C	0.0000000000	-1.2254017980	-0.6397496951
C	0.0000000000	-1.1683582566	0.7406955401
H	0.0000000000	0.0000000000	2.5659444817
H	0.0000000000	2.1600490087	-1.1798151472

S4

H	0.0000000000	0.0000000000	-2.4076969622
H	0.0000000000	-2.1600490087	-1.1798151472

3(¹A_g): UBLYP/cc-pVTZ, E = -230.8637933, S2 = 0.76759

C	0.000000	0.000000	1.350022
C	0.000000	1.214811	0.721496
C	0.000000	1.214811	-0.721496
C	0.000000	0.000000	-1.350022
C	0.000000	-1.214811	-0.721496
C	0.000000	-1.214811	0.721496
H	0.000000	2.172998	1.236663
H	0.000000	2.172998	-1.236663
H	0.000000	-2.172998	-1.236663
H	0.000000	-2.172998	1.236663

3(¹A_g): CCSD(T)/cc-pVTZ, E = -230.43346089, T1: 0.01898

C	0.0000000000	0.0000000000	1.3622921342
C	0.0000000000	1.2112190468	0.7164968432
C	0.0000000000	1.2112190468	-0.7164968432
C	0.0000000000	0.0000000000	-1.3622921342
C	0.0000000000	-1.2112190468	-0.7164968432
C	0.0000000000	-1.2112190468	0.7164968432
H	0.0000000000	2.1629551873	1.2311168634
H	0.0000000000	2.1629551873	-1.2311168634
H	0.0000000000	-2.1629551873	-1.2311168634
H	0.0000000000	-2.1629551873	1.2311168634

3(¹A_g): RS2/cc-pVTZ, E = -230.37571961

C	0.0000000000	0.0000000000	1.3556016146
C	0.0000000000	1.2090338247	0.7198026679
C	0.0000000000	1.2090338247	-0.7198026679
C	0.0000000000	0.0000000000	-1.3556016146
C	0.0000000000	-1.2090338247	-0.7198026679
C	0.0000000000	-1.2090338247	0.7198026679
H	0.0000000000	2.1637131201	1.2241171689
H	0.0000000000	2.1637131201	-1.2241171689
H	0.0000000000	-2.1637131201	-1.2241171689
H	0.0000000000	-2.1637131201	1.2241171689

3(³B_{1u}): UBLYP/cc-pVTZ, E = -230.8566536, S2 = 2.00543

C	0.000000	0.000000	1.322594
C	0.000000	1.237307	0.707774
C	0.000000	1.237307	-0.707774
C	0.000000	0.000000	-1.322594
C	0.000000	-1.237307	-0.707774
C	0.000000	-1.237307	0.707774
H	0.000000	2.170981	1.269334
H	0.000000	2.170981	-1.269334
H	0.000000	-2.170981	-1.269334
H	0.000000	-2.170981	1.269334

3(³B_{1u}): RCCSD(T)/cc-pVTZ, E = -230.42653762, T1: 0.014225

C	0.0000000000	0.0000000000	1.3254760745
C	0.0000000000	1.2360387018	0.7046532877
C	0.0000000000	1.2360387018	-0.7046532877
C	0.0000000000	0.0000000000	-1.3254760745
C	0.0000000000	-1.2360387018	-0.7046532877
C	0.0000000000	-1.2360387018	0.7046532877
H	0.0000000000	2.1627866108	1.2650974687
H	0.0000000000	2.1627866108	-1.2650974687
H	0.0000000000	-2.1627866108	-1.2650974687
H	0.0000000000	-2.1627866108	1.2650974687

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3(³B_{1u}): RS2/cc-pVTZ, E = -230.36705314

C	0.0000000000	0.0000000000	1.3223262052
C	0.0000000000	1.2355035086	0.7042354823
C	0.0000000000	1.2355035086	-0.7042354823
C	0.0000000000	0.0000000000	-1.3223262052
C	0.0000000000	-1.2355035086	-0.7042354823
C	0.0000000000	-1.2355035086	0.7042354823
H	0.0000000000	2.1603194848	1.2635306244
H	0.0000000000	2.1603194848	-1.2635306244
H	0.0000000000	-2.1603194848	-1.2635306244
H	0.0000000000	-2.1603194848	1.2635306244

4(²A₁): UBLYP/cc-pVTZ, E = -230.2337183, S2 = 0.75412

C	0.000000	0.000000	1.778000
C	0.000000	0.883785	0.754565
C	0.000000	1.180718	-0.590214
C	0.000000	0.000000	-1.366184
C	0.000000	-1.180718	-0.590214
C	0.000000	-0.883785	0.754565
H	0.000000	2.187507	-0.993148
H	0.000000	0.000000	-2.456815
H	0.000000	-2.187507	-0.993148

4(²A₁): RCCSD(T)/cc-pVTZ, E = -229.79621429, T1: 0.013139

C	0.000000	0.000000	1.803522
C	0.000000	0.846061	0.746063
C	0.000000	-0.846061	0.746063
C	0.000000	1.175859	-0.594434
C	0.000000	-1.175859	-0.594434
C	0.000000	0.000000	-1.371785
H	0.000000	2.184382	-0.976680
H	0.000000	-2.184382	-0.976680
H	0.000000	0.000000	-2.456600

4(²A₁): RS2/cc-pVTZ, E = -229.74104432

C	0.0000000000	0.0000000000	1.7997283611
C	0.0000000000	0.8551123723	0.7462649057
C	0.0000000000	-0.8551123723	0.7462649057
C	0.0000000000	1.1743359054	-0.5935815387
C	0.0000000000	-1.1743359054	-0.5935815387
C	0.0000000000	0.0000000000	-1.3706451020
H	0.0000000000	2.1800661186	-0.9780718310
H	0.0000000000	-2.1800661186	-0.9780718310
H	0.0000000000	0.0000000000	-2.4532713311

4(²B₂): UBLYP/cc-pVTZ, E = -230.2325303, S2 = 0.80220

C	0.000000	0.000000	1.382215
C	0.000000	1.181023	0.851739
C	0.000000	1.243464	-0.551384
C	0.000000	0.000000	-1.228617
C	0.000000	-1.243464	-0.551384
C	0.000000	-1.181023	0.851739
H	0.000000	2.179944	-1.103797
H	0.000000	0.000000	-2.318247
H	0.000000	-2.179944	-1.103797

4(²B₂): RCCSD(T)/cc-pVTZ, E = -229.79274810, T1: 0.01652188

C	0.000000	0.000000	1.386372
C	0.000000	1.183288	0.848601
C	0.000000	-1.183288	0.848601
C	0.000000	1.241971	-0.552482
C	0.000000	-1.241971	-0.552482
C	0.000000	0.000000	-1.225097

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H	0.000000	2.171414	-1.105867
H	0.000000	-2.171414	-1.105867
H	0.000000	0.000000	-2.309348

4(²B₂): RS2/cc-pVTZ, E = -229.73995281

C	0.0000000000	0.0000000000	1.3962308265
C	0.0000000000	1.1812161177	0.8453819120
C	0.0000000000	-1.1812161177	0.8453819120
C	0.0000000000	1.2407233825	-0.5540372512
C	0.0000000000	-1.2407233825	-0.5540372512
C	0.0000000000	0.0000000000	-1.2260612312
H	0.0000000000	2.1683719253	-1.1062224926
H	0.0000000000	-2.1683719253	-1.1062224926
H	0.0000000000	0.0000000000	-2.3079829315

4(⁴B₂): UBLYP/cc-pVTZ, E = -230.1500018, S2 = 3.75946, v_i = -96.15 1/cm

C	0.000000	0.000000	-1.259254
C	0.000000	1.228166	-0.569670
C	0.000000	-1.228166	-0.569670
C	0.000000	1.207757	0.813333
C	0.000000	-1.207757	0.813333
C	0.000000	0.000000	1.535818
H	0.000000	0.000000	-2.348440
H	0.000000	2.170494	-1.117445
H	0.000000	-2.170494	-1.117445

4(⁴B₂): RCCSD(T)/cc-pVTZ, E = -229.71621218, T1: 0.0153643

C	0.000000	0.000000	1.535551
C	0.000000	1.205847	0.813635
C	0.000000	-1.205847	0.813635
C	0.000000	1.224833	-0.571452
C	0.000000	-1.224833	-0.571452
C	0.000000	0.000000	-1.258222
H	0.000000	2.162073	-1.114330
H	0.000000	-2.162073	-1.114330
H	0.000000	0.000000	-2.341512

4(⁴B₂): RS2/cc-pVTZ, E = -229.66468925

C	0.0000000000	0.0000000000	1.5351572640
C	0.0000000000	1.2059313805	0.8124549371
C	0.0000000000	-1.2059313805	0.8124549371
C	0.0000000000	1.2246508541	-0.5719175552
C	0.0000000000	-1.2246508541	-0.5719175552
C	0.0000000000	0.0000000000	-1.2577097253
H	0.0000000000	2.1596620911	-1.1141494467
H	0.0000000000	-2.1596620911	-1.1141494467
H	0.0000000000	0.0000000000	-2.3387004089

5(²A') : UBLYP/cc-pVTZ, E = -230.2281994, S2 = 0.781831

C	-1.318639	0.807649	0.000000
C	0.000000	1.245836	0.000000
C	-1.198058	-0.580194	0.000000
C	1.199416	0.549798	0.000000
C	-0.166983	-1.317963	0.000000
C	1.152675	-0.872797	0.000000
H	-2.212826	1.420754	0.000000
H	2.153249	1.073912	0.000000
H	2.049111	-1.488643	0.000000

5(²A') : RCCSD(T)/cc-pVTZ, E = -229.790056056, T1: 0.0175167

C	-1.308337	0.795951	0.000000
C	0.000000	1.265469	0.000000

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C	-1.206182	-0.596760	0.000000
C	1.197542	0.549577	0.000000
C	-0.166596	-1.316694	0.000000
C	1.151485	-0.863704	0.000000
H	-2.199804	1.403807	0.000000
H	2.148247	1.067559	0.000000
H	2.044083	-1.474401	0.000000

5(²A'): RS2/cc-pVTZ, E = -229.73641765

C	0.0000000000	-1.3113989430	0.7969297430
C	0.0000000000	0.0027465316	1.2568598870
C	0.0000000000	-1.2065513849	-0.5888195741
C	0.0000000000	1.1969257811	0.5512833927
C	0.0000000000	-0.1602416564	-1.3196256177
C	0.0000000000	1.1512132448	-0.8657772494
H	0.0000000000	-2.2000288907	1.4048977294
H	0.0000000000	2.1450186121	1.0698988608
H	0.0000000000	2.0427547055	-1.4748431716

5(²A', State 2): RS2/cc-pVTZ, E = -229.69512470

C	0.0000000000	-1.2645081627	0.8111216591
C	0.0000000000	0.0249753068	1.3096065604
C	0.0000000000	-1.2561400951	-0.5891313918
C	0.0000000000	1.1844078641	0.5770937706
C	0.0000000000	-0.1453888998	-1.4175377716
C	0.0000000000	1.1090972396	-0.8498529831
H	0.0000000000	-2.1754479387	1.3889566568
H	0.0000000000	2.1591497307	1.0434855598
H	0.0000000000	2.0210829552	-1.4356550602

5(⁴A'): UBLYP/cc-pVTZ, E = -230.161018, S2 = 3.759615

C	-1.260803	0.722024	0.000000
C	0.000000	1.306960	0.000000
C	-1.302924	-0.663049	0.000000
C	1.205197	0.633867	0.000000
C	-0.109269	-1.399063	0.000000
C	1.128794	-0.781282	0.000000
H	-2.175580	1.319702	0.000000
H	2.167253	1.143063	0.000000
H	2.042361	-1.379507	0.000000

5(⁴A'): RCCSD(T)/cc-pVTZ, E = -229.72532457, T1: 0.016564

C	0.0000000000	-1.2456429564	0.7603947798
C	0.0000000000	0.0329589349	1.3067318230
C	0.0000000000	-1.3266694234	-0.6233525222
C	0.0000000000	1.2145365808	0.5919499608
C	0.0000000000	-0.1564317013	-1.3964823674
C	0.0000000000	1.1004695992	-0.8156544046
H	0.0000000000	-2.1356860181	1.3802705039
H	0.0000000000	2.1847089498	1.0715650503
H	0.0000000000	1.9889840344	-1.4373358236

5(⁴A'): RS2/cc-pVTZ, E = -229.67388472

C	0.0000000000	-1.2444966207	0.7612508258
C	0.0000000000	0.0319593532	1.3049838668
C	0.0000000000	-1.3265100666	-0.6234916011
C	0.0000000000	1.2147680049	0.5913414939
C	0.0000000000	-0.1563620670	-1.3956317895
C	0.0000000000	1.1009245903	-0.8141767444
H	0.0000000000	-2.1334315710	1.3791148662
H	0.0000000000	2.1830520234	1.0697537927
H	0.0000000000	1.9873243534	-1.4350577104

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$6(^2A_1)$: UBLYP/cc-pVTZ, E = -230.2144572, S2 = 0.754362

C	1.217372	-0.765842	0.000000
C	-0.034230	-1.405362	0.000000
C	1.252036	0.639251	0.000000
C	-1.079652	-0.518489	0.000000
C	0.000000	1.197678	0.000000
C	-1.317083	0.828572	0.000000
H	-2.234417	1.405705	0.000000
H	2.167436	1.222453	0.000000
H	-0.163678	-2.483008	0.000000

$6(^2A_1)$: RCCSD(T)/cc-pVTZ, E = -229.774136771, T1: 0.021248

C	0.000000	0.000000	-1.428902
C	0.000000	1.206599	-0.723242
C	0.000000	-1.206599	-0.723242
C	0.000000	1.030021	0.642819
C	0.000000	-1.030021	0.642819
C	0.000000	0.000000	1.547493
H	0.000000	0.000000	2.624530
H	0.000000	-2.182053	-1.185498
H	0.000000	2.182053	-1.185498

$6(^2A_1)$: RS2/cc-pVTZ, E = -229.72299868

C	0.0000000000	0.0000000000	-1.4143496636
C	0.0000000000	1.2099119527	-0.7190532534
C	0.0000000000	-1.2099119527	-0.7190532534
C	0.0000000000	1.0517672288	0.6494575381
C	0.0000000000	-1.0517672288	0.6494575381
C	0.0000000000	0.0000000000	1.5344023167
H	0.0000000000	0.0000000000	2.6092578491
H	0.0000000000	-2.1795499383	-1.1894200359
H	0.0000000000	2.1795499383	-1.1894200359

$6(^2B_2)$: UBLYP/cc-pVTZ, E = -230.2126385, S2 = 0.846568, v_i = -264.61 1/cm

C	0.000000	0.000000	1.383825
C	0.000000	1.183924	0.658031
C	0.000000	1.284282	-0.741897
C	0.000000	0.000000	-1.186370
C	0.000000	-1.284282	-0.741897
C	0.000000	-1.183924	0.658031
H	0.000000	0.000000	2.471648
H	0.000000	2.197201	-1.324993
H	0.000000	-2.197201	-1.324993

$6(^2B_2)$: RCCSD(T)/cc-pVTZ, E = -229.77076895, T1: 0.0285762

C	0.000000	0.000000	1.384291
C	0.000000	1.183560	0.657719
C	0.000000	-1.183560	0.657719
C	0.000000	1.285625	-0.737166
C	0.000000	-1.285625	-0.737166
C	0.000000	0.000000	-1.196278
H	0.000000	0.000000	2.465811
H	0.000000	2.191309	-1.320264
H	0.000000	-2.191309	-1.320264

$6(^2B_2)$: RS2/cc-pVTZ, E = -229.72244995

C	0.0000000000	0.0000000000	1.3833082295
C	0.0000000000	1.1828233490	0.6585426927
C	0.0000000000	-1.1828233490	0.6585426927
C	0.0000000000	1.2837455873	-0.7355877014
C	0.0000000000	-1.2837455873	-0.7355877014
C	0.0000000000	0.0000000000	-1.2045021564

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H	0.0000000000	0.0000000000	2.4629084471
H	0.0000000000	2.1886682647	-1.3166112514
H	0.0000000000	-2.1886682647	-1.3166112514

6(⁴B₂): UBLYP/cc-pVTZ, E = -230.1611019, S2 = 3.774553

C	0.000000	1.353439	0.000000
C	1.230331	0.710332	0.000000
C	-1.230331	0.710332	0.000000
C	1.172113	-0.676720	0.000000
C	-1.172113	-0.676720	0.000000
C	0.000000	-1.420663	0.000000
H	0.000000	-2.511175	0.000000
H	-2.174742	1.255588	0.000000
H	2.174742	1.255588	0.000000

6(⁴B₂): RCCSD(T)/cc-pVTZ, E = -229.725733319, T1: 0.015914

C	0.000000	0.000000	1.420647
C	0.000000	1.172993	0.677218
C	0.000000	-1.172993	0.677218
C	0.000000	1.230318	-0.710303
C	0.000000	-1.230318	-0.710303
C	0.000000	0.000000	-1.354456
H	0.000000	0.000000	2.503753
H	0.000000	2.168268	-1.251944
H	0.000000	-2.168268	-1.251944

6(⁴B₂): RS2/cc-pVTZ, E = -229.67459113

C	0.0000000000	0.0000000000	1.4200562667
C	0.0000000000	1.1718440420	0.6765527564
C	0.0000000000	-1.1718440420	0.6765527564
C	0.0000000000	1.2298171976	-0.7100469629
C	0.0000000000	-1.2298171976	-0.7100469629
C	0.0000000000	0.0000000000	-1.3531362816
H	0.0000000000	0.0000000000	2.5010311774
H	0.0000000000	2.1659661732	-1.2505383748
H	0.0000000000	-2.1659661732	-1.2505383748

7(²A₁): UBLYP/cc-pVTZ, E = -231.5405068, S2 = 0.754689

C	0.000000	0.000000	1.400899
C	0.000000	1.228256	0.775363
C	0.000000	-1.228256	0.775363
C	0.000000	1.217215	-0.634868
C	0.000000	-1.217215	-0.634868
C	0.000000	0.000000	-1.327926
H	0.000000	2.167315	1.325927
H	0.000000	-2.167315	1.325927
H	0.000000	2.160406	-1.179802
H	0.000000	-2.160406	-1.179802
H	0.000000	0.000000	-2.416024

7(²A₁): RCCSD(T)/cc-pVTZ, E = -231.11716269, T1: 0.013050

C	0.0000000000	0.0000000000	1.4019664338
C	0.0000000000	1.2280694091	0.7713778033
C	0.0000000000	-1.2280694091	0.7713778033
C	0.0000000000	1.2150865285	-0.6334597337
C	0.0000000000	-1.2150865285	-0.6334597337
C	0.0000000000	0.0000000000	-1.3254931069
H	0.0000000000	2.1602316618	1.3215034736
H	0.0000000000	-2.1602316618	1.3215034736
H	0.0000000000	2.1517501498	-1.1784358254
H	0.0000000000	-2.1517501498	-1.1784358254
H	0.0000000000	0.0000000000	-2.4082557626

11(¹A') : BLYP/cc-pVTZ, E = -344.2850567

C	-1.567027	1.952754	0.000000
C	-2.269732	0.634039	0.000000
C	-0.228423	1.740734	0.000000
C	-1.347795	-0.357032	0.000000
C	0.000000	0.277165	0.000000
C	1.201252	-0.336509	0.000000
C	1.828743	-1.475465	0.000000
O	2.582568	-2.386344	0.000000
H	0.568106	2.474455	0.000000
H	-2.072097	2.913459	0.000000
H	-3.348892	0.516857	0.000000
H	-1.509759	-1.428130	0.000000

12(¹A') : BLYP/cc-pVTZ, E = -344.2901006

C	-1.402803	0.848025	0.000000
C	-1.994788	-0.417499	0.000000
C	-1.234771	-1.621359	0.000000
C	0.162335	-1.631149	0.000000
C	0.000000	0.826627	0.000000
C	0.746294	-0.355486	0.000000
C	1.449285	0.914956	0.000000
O	2.471204	1.560102	0.000000
H	-1.996978	1.758739	0.000000
H	-3.080549	-0.498054	0.000000
H	-1.774420	-2.566952	0.000000
H	0.728998	-2.559231	0.000000

13(¹A₁) : BLYP/cc-pVTZ, E = -230.8517795

C	0.000000	0.730937	-1.270300
C	0.000000	-0.730937	-1.270300
C	0.000000	1.194497	0.010830
C	0.000000	-1.194497	0.010830
C	0.000000	0.000000	0.901560
C	0.000000	0.000000	2.213914
H	0.000000	1.355665	-2.158265
H	0.000000	-1.355665	-2.158265
H	0.000000	2.214727	0.368665
H	0.000000	-2.214727	0.368665

13(¹A₁) : CCSD(T)/cc-pVTZ, E = -230.42770083, T1: 0.0156795

C	0.0000000000	0.7335173586	-1.2680039709
C	0.0000000000	-0.7335173586	-1.2680039709
C	0.0000000000	1.1902467998	0.0119167184
C	0.0000000000	-1.1902467998	0.0119167184
C	0.0000000000	0.0000000000	0.8947291755
C	0.0000000000	0.0000000000	2.2125139608
H	0.0000000000	1.3543317816	-2.1523427838
H	0.0000000000	-1.3543317816	-2.1523427838
H	0.0000000000	2.2087118572	0.3634754681
H	0.0000000000	-2.2087118572	0.3634754681

(Z)-**26**(¹A₁) : BLYP/cc-pVTZ, E = -230.8854207

C	0.000000	0.681058	1.072534
C	0.000000	-0.681058	1.072534
C	0.000000	1.509878	-0.073206
C	0.000000	-1.509878	-0.073206
C	0.000000	-2.261442	-1.026359
C	0.000000	2.261442	-1.026359
H	0.000000	-2.906655	-1.875370
H	0.000000	-1.189121	2.037556
H	0.000000	2.906655	-1.875370

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H 0.000000 1.189121 2.037556

(E)-26(¹A_g): BLYP/cc-pVTZ, E = -230.8864967

C 0.000000 0.680461 0.000000
 C 0.000000 -0.680461 0.000000
 C 1.169722 1.475593 0.000000
 C -1.169722 -1.475593 0.000000
 C -2.148446 -2.194236 0.000000
 C 2.148446 2.194236 0.000000
 H -3.014898 -2.815923 0.000000
 H 0.954057 -1.209552 0.000000
 H 3.014898 2.815923 0.000000
 H -0.954057 1.209552 0.000000

41(¹A₁): CCSD(T)/cc-pVTZ, E = -626.97819796, T1: 0.01335678

C 0.0000000000 1.4488004037 -0.6070889396
 C 0.0000000000 0.7073092054 0.5794247136
 C 0.0000000000 0.6298094226 -1.7172452204
 C 0.0000000000 -0.7073092054 0.5794247136
 C 0.0000000000 -0.6298094226 -1.7172452204
 C 0.0000000000 -1.4488004037 -0.6070889396
 F 0.0000000000 2.7741089761 -0.5950586145
 F 0.0000000000 1.3307683334 1.7562460609
 F 0.0000000000 -1.3307683334 1.7562460609
 F 0.0000000000 -2.7741089761 -0.5950586145

41(³B₂): RCCSD(T)/cc-pVTZ, E = -626.91016576, T1: 0.01388686

C 0.0000000000 1.4063670905 -0.5997501085
 C 0.0000000000 0.6961025173 0.6084870935
 C 0.0000000000 0.7000980476 -1.7864364949
 C 0.0000000000 -0.6961025173 0.6084870935
 C 0.0000000000 -0.7000980476 -1.7864364949
 C 0.0000000000 -1.4063670905 -0.5997501085
 F 0.0000000000 2.7373610433 -0.5709668423
 F 0.0000000000 1.3531212476 1.7649443522
 F 0.0000000000 -1.3531212476 1.7649443522
 F 0.0000000000 -2.7373610433 -0.5709668423

42(¹A₁): CCSD(T)/cc-pVTZ, E = -626.96000972, T1: 0.01330597

C 0.0000000000 0.0000000000 1.8929562435
 C 0.0000000000 0.9539255622 0.9497407144
 C 0.0000000000 1.1655027434 -0.4034625937
 C 0.0000000000 0.0000000000 -1.1786337497
 C 0.0000000000 -1.1655027434 -0.4034625937
 C 0.0000000000 -0.9539255622 0.9497407144
 F 0.0000000000 0.0000000000 3.2068951710
 F 0.0000000000 2.3793348434 -0.9536042530
 F 0.0000000000 0.0000000000 -2.5010564001
 F 0.0000000000 -2.3793348434 -0.9536042530

42(³B₂): RCCSD(T)/cc-pVTZ, E = -626.91488404, T1: 0.0138712

C 0.0000000000 0.0000000000 1.7416882511
 C 0.0000000000 1.1826366014 1.0196684414
 C 0.0000000000 1.2127239600 -0.3586193442
 C 0.0000000000 0.0000000000 -1.0581135437
 C 0.0000000000 -1.2127239600 -0.3586193442
 C 0.0000000000 -1.1826366014 1.0196684414
 F 0.0000000000 0.0000000000 3.0734813003
 F 0.0000000000 2.3537684302 -1.0418948598
 F 0.0000000000 0.0000000000 -2.3898554826
 F 0.0000000000 -2.3537684302 -1.0418948598

43(¹A_g): CCSD(T)/cc-pVTZ, E = -626.92555110, T1: 0.0203048

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C	0.0000000000	0.0000000000	1.4351114399
C	0.0000000000	1.1813644938	0.7163303275
C	0.0000000000	1.1813644938	-0.7163303275
C	0.0000000000	0.0000000000	-1.4351114399
C	0.0000000000	-1.1813644938	-0.7163303275
C	0.0000000000	-1.1813644938	0.7163303275
F	0.0000000000	2.3793502383	-1.2944048885
F	0.0000000000	2.3793502383	1.2944048885
F	0.0000000000	-2.3793502383	1.2944048885
F	0.0000000000	-2.3793502383	-1.2944048885

43(³B_{1u}): RCCSD(T)/cc-pVTZ, E = -626.92111337, T1: 0.01442001

C	0.0000000000	0.0000000000	1.3339296743
C	0.0000000000	1.2241267961	0.7022222631
C	0.0000000000	1.2241267961	-0.7022222631
C	0.0000000000	0.0000000000	-1.3339296743
C	0.0000000000	-1.2241267961	-0.7022222631
C	0.0000000000	-1.2241267961	0.7022222631
F	0.0000000000	2.3744083924	-1.3717390798
F	0.0000000000	2.3744083924	1.3717390798
F	0.0000000000	-2.3744083924	1.3717390798
F	0.0000000000	-2.3744083924	-1.3717390798

45(¹A₁): BLYP/cc-pVTZ, E = -741.3726688

C	-0.003390	1.453886	0.000000
C	1.184867	0.710221	0.000000
C	1.184867	-0.710196	0.000000
C	-0.003390	-1.453876	0.000000
F	0.045498	2.799883	0.000000
F	2.374896	1.336626	0.000000
F	2.374904	-1.336585	0.000000
F	0.045530	-2.799870	0.000000
C	-1.168885	0.706155	0.000000
C	-1.168880	-0.706148	0.000000
C	-2.435562	-0.000028	0.000000
O	-3.638152	-0.000072	0.000000

46(¹A') : BLYP/cc-pVTZ, E = -741.3577467

C	1.302010	-1.234773	0.000000
C	-0.143343	-1.639855	0.000000
C	1.377140	0.115456	0.000000
C	-0.902563	-0.523874	0.000000
C	0.000000	0.660021	0.000000
C	-0.343177	1.958526	0.000000
F	2.475381	0.885715	0.000000
F	2.284296	-2.137977	0.000000
F	-0.513710	-2.923002	0.000000
F	-2.241080	-0.417798	0.000000
C	-1.389596	2.739859	0.000000
O	-2.180850	3.610675	0.000000

47(¹A₁): BLYP/cc-pVTZ, E = -627.9125138

C	0.000000	0.737688	-0.835408
C	0.000000	-0.737688	-0.835408
C	0.000000	1.186711	0.442734
C	0.000000	-1.186711	0.442734
C	0.000000	0.000000	1.344635
C	0.000000	0.000000	2.665658
F	0.000000	2.451454	0.887403
F	0.000000	1.459228	-1.962384
F	0.000000	-1.459228	-1.962384
F	0.000000	-2.451454	0.887403

48(¹A'): BLYP/cc-pVTZ, E = -330.1832556
 C 0.000000 0.960856 0.000000
 C 1.109262 0.087291 0.000000
 C -1.244952 0.351750 0.000000
 C 0.930136 -1.306526 0.000000
 C -1.298573 -0.903377 0.000000
 C -0.358561 -1.907379 0.000000
 F 0.197571 2.302967 0.000000
 H 2.109949 0.513668 0.000000
 H 1.804375 -1.956363 0.000000
 H -0.516339 -2.979702 0.000000

49a(¹A'): BLYP/cc-pVTZ, E = -237.8102056
 C 1.220722 0.563647 0.000000
 C 0.859777 -0.848649 0.000000
 C 0.000000 1.146300 0.000000
 C -0.474632 -1.303309 0.000000
 C -1.258129 0.964868 0.000000
 C -1.579266 -0.417715 0.000000
 H 1.659794 -1.592148 0.000000
 H -0.658112 -2.378410 0.000000
 H -2.601293 -0.798247 0.000000
 Li 2.996259 1.379316 0.000000

49b(¹A'): BLYP/cc-pVTZ, E = -237.8154087
 C 1.286503 0.960211 0.000000
 C 0.000000 1.141231 0.000000
 C -1.319713 0.772604 0.000000
 C -1.436538 -0.628097 0.000000
 C -0.192688 -1.291526 0.000000
 C 1.007923 -0.584248 0.000000
 H -2.153881 1.466293 0.000000
 H -2.403293 -1.134457 0.000000
 H -0.144275 -2.380528 0.000000
 Li 2.876175 -0.057454 0.000000

(Z)-**63**(¹A₁): BLYP/cc-pVTZ, E = -627.9273336
 C 0.000000 0.680147 1.009643
 C 0.000000 -0.680147 1.009643
 C 0.000000 1.507584 -0.129867
 C 0.000000 -1.507584 -0.129867
 C 0.000000 -2.266172 -1.071491
 C 0.000000 2.266172 -1.071491
 F 0.000000 3.056342 -2.087613
 F 0.000000 -3.056342 -2.087613
 F 0.000000 1.323514 2.215423
 F 0.000000 -1.323514 2.215423

(Z)-**64**(¹A₁): BLYP/cc-pVTZ, E = -429.4238675
 C 0.000000 0.680902 -0.411213
 C 0.000000 -0.680902 -0.411213
 C 0.000000 1.507584 0.728100
 C 0.000000 -1.507584 0.728100
 C 0.000000 -2.253458 1.684399
 C 0.000000 2.253458 1.684399
 H 0.000000 2.901820 2.531603
 H 0.000000 -2.901820 2.531603
 F 0.000000 1.323275 -1.615480
 F 0.000000 -1.323275 -1.615480

(Z)-**65**(¹A₁): BLYP/cc-pVTZ, E = -429.388151
 C 0.000000 0.680478 1.668510
 C 0.000000 -0.680478 1.668510

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C	0.000000	1.508027	0.518697
C	0.000000	-1.508027	0.518697
C	0.000000	-2.254600	-0.433136
C	0.000000	2.254600	-0.433136
F	0.000000	3.037392	-1.461978
F	0.000000	-3.037392	-1.461978
H	0.000000	1.188067	2.633376
H	0.000000	-1.188067	2.633376

66(¹A_g): UBLYP/cc-pVTZ, E = -429.3983468, S2 = 0.977513

C	0.000000	1.344284	0.696551
C	0.000000	0.714427	1.915224
C	0.000000	-0.714427	1.915224
C	0.000000	-1.344284	0.696551
C	0.000000	-0.710329	-0.525969
C	0.000000	0.710329	-0.525969
F	0.000000	1.369807	-1.708384
F	0.000000	-1.369807	-1.708384
H	0.000000	-1.252983	2.860625
H	0.000000	1.252983	2.860625

71(²A₁): UBLYP/cc-pVTZ, E = -528.0190855, S2 = 0.755058

C	0.000000	0.000000	1.508087
C	0.000000	0.999875	0.602862
C	0.000000	1.182750	-0.760346
C	0.000000	0.000000	-1.489421
C	0.000000	-1.182750	-0.760346
C	0.000000	-0.999875	0.602862
F	0.000000	-2.410175	-1.324552
F	0.000000	2.410175	-1.324552
F	0.000000	0.000000	2.846637

71(²A₁): RCCSD(T)/cc-pVTZ, E = -527.143983919, T1: 0.0167118

C	0.000000	0.000000	1.501146
C	0.000000	1.013731	0.609818
C	0.000000	-1.013731	0.609818
C	0.000000	1.180502	-0.756844
C	0.000000	-1.180502	-0.756844
C	0.000000	0.000000	-1.484209
F	0.000000	-2.386932	-1.316433
F	0.000000	2.386932	-1.316433
F	0.000000	0.000000	2.817609

71(²B₂): UBLYP/cc-pVTZ, E = -528.0159188, S2 = 0.844082, v_i = -296.61 1/cm

C	0.000000	0.000000	1.387431
C	0.000000	1.189985	0.673964
C	0.000000	1.274604	-0.697431
C	0.000000	0.000000	-1.173474
C	0.000000	-1.274604	-0.697431
C	0.000000	-1.189985	0.673964
F	0.000000	0.000000	2.741923
F	0.000000	-2.403124	-1.426635
F	0.000000	2.403124	-1.426635

71(²B₂): RCCSD(T)/cc-pVTZ, E = -527.13934393, T1: 0.0224326

C	0.0000000000	0.0000000000	1.3605867387
C	0.0000000000	1.1925531346	0.6523758242
C	0.0000000000	1.2705320557	-0.7187792424
C	0.0000000000	0.0000000000	-1.2117953500
C	0.0000000000	-1.2705320557	-0.7187792424
C	0.0000000000	-1.1925531346	0.6523758242
F	0.0000000000	0.0000000000	2.6939278396

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F	0.0000000000	2.3810010721	-1.4365011960
F	0.0000000000	-2.3810010721	-1.4365011960

71(⁴B₂): RCCSD(T)/cc-pVTZ, E = -527.09110059, T1: 0.0141007

C	0.0000000000	0.0000000000	1.4013426222
C	0.0000000000	1.1889720806	0.6864449090
C	0.0000000000	-1.1889720806	0.6864449090
C	0.0000000000	1.2136173111	-0.7007035597
C	0.0000000000	-1.2136173111	-0.7007035597
C	0.0000000000	0.0000000000	-1.3729277061
F	0.0000000000	2.3669760758	-1.3665965533
F	0.0000000000	-2.3669760758	-1.3665965533
F	0.0000000000	0.0000000000	2.7331419119

75(¹A'): BLYP/cc-pVTZ, E = -246.962748

N	-1.157107	0.570644	0.000000
C	0.000000	1.235030	0.000000
C	-1.187114	-0.784150	0.000000
C	1.295408	0.627835	0.000000
C	0.074351	-1.375276	0.000000
C	1.169742	-0.746449	0.000000
H	-0.067196	2.323378	0.000000
H	2.202822	1.225485	0.000000
H	-2.150203	-1.285311	0.000000

75(¹A'): CCSD(T)/cc-pVTZ, E = -246.50545007, T1: 0.0165276

N	0.0000000000	-1.1635593586	0.5713169257
C	0.0000000000	0.0041604301	1.2292331374
C	0.0000000000	-1.1808247674	-0.7758392625
C	0.0000000000	1.2908733674	0.6332876228
C	0.0000000000	0.0741972620	-1.3827127916
C	0.0000000000	1.1667774504	-0.7444034677
H	0.0000000000	-0.0673884253	2.3112338317
H	0.0000000000	2.1957197236	1.2238499181
H	0.0000000000	-2.1392526821	-1.2747799140

75(³A'): RCCSD(T)/cc-pVTZ, E = -246.44337734, T1: 0.017448

N	-1.176269	0.615782	0.000000
C	0.000000	1.251642	0.000000
C	-1.156286	-0.734668	0.000000
C	1.252669	0.610303	0.000000
C	0.026805	-1.456365	0.000000
C	1.247473	-0.769474	0.000000
H	-0.045435	2.335438	0.000000
H	2.171728	1.183520	0.000000
H	-2.116379	-1.238064	0.000000

76(¹A'): BLYP/cc-pVTZ, E = -246.9535877

C	1.285569	-0.535763	0.000000
C	0.049149	-1.234021	0.000000
C	1.236483	0.889113	0.000000
C	-1.175193	-0.554676	0.000000
C	0.000000	1.200074	0.000000
N	-1.215081	0.839560	0.000000
H	2.226993	-1.085958	0.000000
H	0.040818	-2.321916	0.000000
H	-2.138292	-1.057404	0.000000

76(¹A'): CCSD(T)/cc-pVTZ, E = -246.49645636, T1: 0.023375

C	0.0000000000	1.2931683969	-0.5443363475
C	0.0000000000	0.0557892192	-1.2295264709
C	0.0000000000	1.2199039804	0.8696587199
C	0.0000000000	-1.1649673323	-0.5404831649

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C	0.0000000000	-0.0065448242	1.2054768788
N	0.0000000000	-1.2350994585	0.8404804880
H	0.0000000000	2.2282664466	-1.0935076882
H	0.0000000000	0.0355037153	-2.3119119296
H	0.0000000000	-2.1155741433	-1.0568414856

76(¹A', State 2): BLYP/cc-pVTZ, E = -246.9093053

C	-1.310910	1.405542	0.000000
N	-1.018141	-0.067749	0.000000
C	-0.347688	-1.227902	0.000000
C	1.051748	-0.984951	0.000000
C	1.267204	0.402273	0.000000
C	0.000000	0.984922	0.000000
H	-0.873359	-2.176793	0.000000
H	1.822451	-1.751703	0.000000
H	2.215774	0.923431	0.000000

76(¹A', State 2): CCSD(T)/cc-pVTZ, E = -246.45803880, T1: 0.013693

C	0.0000000000	-1.3189089324	1.3855001158
N	0.0000000000	-1.0012713996	-0.0600183906
C	0.0000000000	-0.3456918127	-1.2234782642
C	0.0000000000	1.0499411183	-0.9833452500
C	0.0000000000	1.2692545974	0.4010550495
C	0.0000000000	0.0014406334	0.9797448386
H	0.0000000000	-0.8747419797	-2.1638007284
H	0.0000000000	1.8141989506	-1.7489953966
H	0.0000000000	2.2128578247	0.9204080259

76(³A'): UBLYP/cc-pVTZ, E = -246.9214654, S2 = 2.007088

N	-1.199395	0.663548	0.000000
C	-1.328658	-0.621753	0.000000
C	0.000000	1.290185	0.000000
C	-0.196972	-1.428513	0.000000
C	1.173879	0.538355	0.000000
C	1.066369	-0.871777	0.000000
H	0.000051	2.378054	0.000000
H	2.144972	1.030092	0.000000
H	1.963040	-1.491960	0.000000

76(³A'): RCCSD(T)/cc-pVTZ, E = -246.46028233, T1: 0.0260743

N	0.0000000000	-1.2111139633	0.6738735406
C	0.0000000000	-1.3185094256	-0.6069438460
C	0.0000000000	-0.0017810191	1.2823165550
C	0.0000000000	-0.1880714424	-1.4296680095
C	0.0000000000	1.1689721442	0.5361344268
C	0.0000000000	1.0717511734	-0.8730731498
H	0.0000000000	0.0060818771	2.3645193825
H	0.0000000000	2.1330423661	1.0287123071
H	0.0000000000	1.9629142896	-1.4896402066

77(¹A'): BLYP/cc-pVTZ, E = -246.9534725

N	-1.141302	0.718568	0.000000
C	-1.216024	-0.634203	0.000000
C	0.000000	1.254143	0.000000
C	0.021285	-1.313768	0.000000
C	1.327627	0.787558	0.000000
C	1.190123	-0.577676	0.000000
H	-2.187176	-1.128453	0.000000
H	0.021229	-2.401914	0.000000
H	2.217000	1.404060	0.000000

77(¹A'): CCSD(T)/cc-pVTZ, E = -246.49601841, T1: 0.031157

N	0.0000000000	-1.1552877479	0.7232918315
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C	0.0000000000	-1.2046937485	-0.6294469661
C	0.0000000000	-0.0000972410	1.2516009069
C	0.0000000000	0.0161564298	-1.3165669955
C	0.0000000000	1.3234281535	0.7851319484
C	0.0000000000	1.1920139570	-0.5808888297
H	0.0000000000	-2.1703162047	-1.1227722038
H	0.0000000000	0.0222376235	-2.3986141599
H	0.0000000000	2.2093207784	1.3965794682

77(³A') : UBLYP/cc-pVTZ, E = -246.9145211, S2 = 2.009466

N	-1.191321	0.652319	0.000000
C	0.000000	1.311583	0.000000
C	-1.206709	-0.638042	0.000000
C	1.219239	0.621880	0.000000
C	-0.073191	-1.462023	0.000000
C	1.117063	-0.761833	0.000000
H	-0.038339	2.400318	0.000000
H	2.168391	1.153049	0.000000
H	-0.129213	-2.548997	0.000000

77(³A') : RCCSD(T)/cc-pVTZ, E = -246.45669124, T1: 0.0200348

N	0.0000000000	-1.2004505034	0.6638299056
C	0.0000000000	-0.0024181579	1.3026289929
C	0.0000000000	-1.1931667583	-0.6295972964
C	0.0000000000	1.2154642441	0.6205968633
C	0.0000000000	-0.0679185789	-1.4613676542
C	0.0000000000	1.1239840958	-0.7653880741
H	0.0000000000	-0.0343375972	2.3855793363
H	0.0000000000	2.1565701466	1.1527908395
H	0.0000000000	-0.1318068908	-2.5408189129

78(¹A₁) : BLYP/cc-pVTZ, E = -246.9329531

N	0.000000	0.000000	1.472831
C	0.000000	1.106142	0.683460
C	0.000000	-1.106142	0.683460
C	0.000000	0.969450	-0.686959
C	0.000000	-0.969450	-0.686959
C	0.000000	0.000000	-1.644966
H	0.000000	2.080649	1.166370
H	0.000000	-2.080649	1.166370
H	0.000000	0.000000	-2.730777

78(¹A₁) : CCSD(T)/cc-pVTZ, E = -246.47830161, T1: 0.0151413

N	0.0000000000	0.0000000000	1.4599051929
C	0.0000000000	1.1030170650	0.6803899756
C	0.0000000000	-1.1030170650	0.6803899756
C	0.0000000000	0.9998214560	-0.6965402241
C	0.0000000000	-0.9998214560	-0.6965402241
C	0.0000000000	0.0000000000	-1.6299749477
H	0.0000000000	2.0694061833	1.1666285072
H	0.0000000000	-2.0694061833	1.1666285072
H	0.0000000000	0.0000000000	-2.7080567626

78(³B₂) : UBLYP/cc-pVTZ, E = -246.9140503, S2 = 2.011613

N	0.000000	0.000000	1.324337
C	0.000000	1.180931	0.670981
C	0.000000	-1.180931	0.670981
C	0.000000	1.174472	-0.716556
C	0.000000	-1.174472	-0.716556
C	0.000000	0.000000	-1.455218
H	0.000000	2.083796	1.276880
H	0.000000	-2.083796	1.276880
H	0.000000	0.000000	-2.545907

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78(³B₂): RCCSD(T)/cc-pVTZ, E = -246.45146479, T1: 0.0239616

N	0.0000000000	0.0000000000	1.3447790463
C	0.0000000000	1.1674709326	0.6723856824
C	0.0000000000	-1.1674709326	0.6723856824
C	0.0000000000	1.1667461793	-0.7138670607
C	0.0000000000	-1.1667461793	-0.7138670607
C	0.0000000000	0.0000000000	-1.4613842030
H	0.0000000000	2.0720259707	1.2650868459
H	0.0000000000	-2.0720259707	1.2650868459
H	0.0000000000	0.0000000000	-2.5447837785

79(¹A'): BLYP/cc-pVTZ, E = -246.9407628

C	0.000000	1.329603	0.000000
N	-1.097556	0.756665	0.000000
C	-1.282332	-0.665005	0.000000
C	-0.112964	-1.345131	0.000000
C	1.114665	-0.727418	0.000000
C	1.235457	0.708452	0.000000
H	-2.307616	-1.010343	0.000000
H	2.054035	-1.279820	0.000000
H	2.207518	1.190505	0.000000

79(¹A'): BCCD(T)/cc-pVTZ, E = -246.47784176

C	0.0000000000	-0.0029361381	1.3316521886
N	0.0000000000	-1.1142176791	0.7565598408
C	0.0000000000	-1.2765498096	-0.6480458343
C	0.0000000000	-0.1095351197	-1.3362451019
C	0.0000000000	1.1263578822	-0.7256491851
C	0.0000000000	1.2304166725	0.6962165374
H	0.0000000000	-2.2908102813	-1.0117060479
H	0.0000000000	2.0528800696	-1.2875166587
H	0.0000000000	2.1956014035	1.1822422610

79(³A'): RCCSD(T)/cc-pVTZ, E = -246.45718701, T1: 0.019003

C	0.0000000000	-0.0104520930	1.3040890168
N	0.0000000000	-1.1976585474	0.7824670182
C	0.0000000000	-1.2717620242	-0.5752328791
C	0.0000000000	-0.0969156327	-1.2984857070
C	0.0000000000	1.1754353625	-0.7393200490
C	0.0000000000	1.2312650780	0.6572008326
H	0.0000000000	-2.2536898478	-1.0291086501
H	0.0000000000	2.0713011577	-1.3484817656
H	0.0000000000	2.1636835468	1.2043801829

80(¹A₁): BLYP/cc-pVTZ, E = -246.9208965

N	0.000000	0.000000	1.682568
C	0.000000	0.968216	0.737295
C	0.000000	1.162094	-0.627459
C	0.000000	0.000000	-1.418098
C	0.000000	-1.162094	-0.627459
C	0.000000	-0.968216	0.737295
H	0.000000	2.168527	-1.037686
H	0.000000	0.000000	-2.512047
H	0.000000	-2.168527	-1.037686

80(¹A₁): CCSD(T)/cc-pVTZ, E = -246.469992623, T1: 0.019793

N	0.000000	0.000000	1.642715
C	0.000000	1.011745	0.748792
C	0.000000	-1.011745	0.748792
C	0.000000	1.166849	-0.625941
C	0.000000	-1.166849	-0.625941
C	0.000000	0.000000	-1.398397
H	0.000000	2.161508	-1.048996

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H	0.000000	-2.161508	-1.048996
H	0.000000	0.000000	-2.484847

80(¹A₁, State 2): BLYP/cc-pVTZ, E = -246.9316641

N	0.000000	0.000000	1.194761
C	0.000000	1.199213	0.866736
C	0.000000	1.244439	-0.570066
C	0.000000	0.000000	-1.232930
C	0.000000	-1.244439	-0.570066
C	0.000000	-1.199213	0.866736
H	0.000000	2.190139	-1.101955
H	0.000000	0.000000	-2.321879
H	0.000000	-2.190139	-1.101955

80(¹A₁, State 2): CCSD(T)/cc-pVTZ, E = -246.4674993855, T1: 0.0260878

N	0.000000	0.000000	1.185041
C	0.000000	1.201176	0.865372
C	0.000000	-1.201176	0.865372
C	0.000000	1.243695	-0.566688
C	0.000000	-1.243695	-0.566688
C	0.000000	0.000000	-1.227132
H	0.000000	2.181248	-1.103062
H	0.000000	-2.181248	-1.103062
H	0.000000	0.000000	-2.310581

80(³B₂): UBLYP/cc-pVTZ, E = -246.9290395, S2 = 2.00931

N	0.000000	0.000000	1.447744
C	0.000000	1.129607	0.790108
C	0.000000	1.219294	-0.599232
C	0.000000	0.000000	-1.300704
C	0.000000	-1.219294	-0.599232
C	0.000000	-1.129607	0.790108
H	0.000000	2.175265	-1.114608
H	0.000000	0.000000	-2.391281
H	0.000000	-2.175265	-1.114608

80(³B₂): RCCSD(T)/cc-pVTZ, E = -246.4695558367, T1: 0.0230203

N	0.000000	0.000000	1.457058
C	0.000000	1.118952	0.785862
C	0.000000	-1.118952	0.785862
C	0.000000	1.216121	-0.601501
C	0.000000	-1.216121	-0.601501
C	0.000000	0.000000	-1.300910
H	0.000000	2.168894	-1.110432
H	0.000000	-2.168894	-1.110432
H	0.000000	0.000000	-2.385407

86(¹A') : BLYP/cc-pVTZ, E = -246.913214

C	-0.516393	2.111338	0.000000
C	0.000000	0.910112	0.000000
C	-1.119679	-0.158997	0.000000
C	1.220671	0.124355	0.000000
N	-0.570231	-1.331987	0.000000
C	0.830338	-1.184514	0.000000
H	2.221488	0.536109	0.000000
H	1.463140	-2.065090	0.000000
H	-2.182636	0.039127	0.000000

(Z)-**88**(¹A') : BLYP/cc-pVTZ, E = -246.9943661

N	-1.340399	-2.052837	0.000000
C	0.000000	1.239617	0.000000
C	-1.157752	0.528172	0.000000
C	-1.233794	-0.891442	0.000000

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C	1.305181	0.698453	0.000000
C	2.441980	0.275579	0.000000
H	3.433786	-0.117735	0.000000
H	-0.076005	2.327650	0.000000
H	-2.108679	1.057677	0.000000

(Z)-**90**(¹A'): BLYP/cc-pVTZ, E = -246.9592918

C	0.000000	1.199997	0.000000
C	-1.160155	0.499301	0.000000
C	1.300123	0.647594	0.000000
N	-1.229699	-0.873778	0.000000
C	-1.338660	-2.053330	0.000000
C	2.430788	0.208866	0.000000
H	-2.120831	1.008642	0.000000
H	3.418755	-0.193453	0.000000
H	-0.082607	2.286696	0.000000

92a(¹A'): BLYP/cc-pVTZ, E = -246.9152064

C	-0.723606	-2.022724	0.000000
C	-1.312869	-0.859239	0.000000
C	-1.182055	0.578936	0.000000
C	0.000000	1.246568	0.000000
C	1.265637	0.604483	0.000000
H	-2.335108	-1.332987	0.000000
H	-2.101054	1.159587	0.000000
H	0.001503	2.334475	0.000000
H	2.307432	0.078684	0.000000

92b(¹A'): BLYP/cc-pVTZ, E = -246.8810373

C	-1.266605	-0.889653	0.000000
C	-1.174008	0.554657	0.000000
C	-0.524065	-1.968460	0.000000
C	0.000000	1.228498	0.000000
C	2.267848	0.042399	0.000000
N	1.215495	0.590117	0.000000
H	-2.268327	-1.380928	0.000000
H	-2.094696	1.130712	0.000000
H	0.035538	2.314751	0.000000

(Z)-**97**(¹A'): BLYP/cc-pVTZ, E = -246.9332637

N	-1.130148	0.589644	0.000000
C	0.000000	1.238630	0.000000
C	-1.219928	-0.735522	0.000000
C	1.302655	0.671586	0.000000
C	2.424271	0.208404	0.000000
C	-1.471804	-1.927233	0.000000
H	3.405223	-0.211743	0.000000
H	-0.068546	2.328709	0.000000
H	-1.636808	-2.979672	0.000000

TS[1-13](¹A'): BLYP/cc-pVTZ, E = -230.849787, $\nu_i = -233.83$ 1/cm

C	-0.312235	-1.306675	0.000000
C	1.086692	-0.987711	0.000000
C	1.267886	0.379429	0.000000
C	0.000000	1.001588	0.000000
C	-1.106031	1.668375	0.000000
H	-0.720600	-2.313037	0.000000
H	1.888617	-1.719516	0.000000
H	2.199286	0.931109	0.000000
C	-1.129449	-0.202276	0.000000
H	-2.208479	-0.214941	0.000000

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TS[1-13](¹A'): CCSD(T)/cc-pVTZ, E = -230.42533997, T1: 0.012813

C	0.0000000000	-0.3141848343	-1.2887360648
C	0.0000000000	1.0840899694	-0.9822323966
C	0.0000000000	1.2785248882	0.3793402395
C	0.0000000000	0.0201357934	1.0141459533
C	0.0000000000	-1.1238761198	1.6113315159
H	0.0000000000	-0.7269941975	-2.2874402142
H	0.0000000000	1.8775953894	-1.7160812119
H	0.0000000000	2.2099330287	0.9212555545
C	0.0000000000	-1.1321601154	-0.1856639670
H	0.0000000000	-2.2073768020	-0.2295744086

TS[41-47](¹A): BLYP/cc-pVTZ, E = -627.9011369, v_i = -234.04 1/cm

C	-0.554455	0.832215	0.154292
C	0.852815	0.693528	-0.038177
C	1.156726	-0.633897	-0.258942
C	-0.049919	-1.408561	-0.172080
C	-0.820442	-2.154000	0.581782
C	-1.213300	-0.394921	0.123666
F	2.368105	-1.187187	-0.102819
F	1.740589	1.685667	0.117939
F	-1.199783	2.001845	0.033509
F	-2.489861	-0.456568	-0.308990

TS[3-26](¹A₁): BLYP/cc-pVTZ, E = -230.8397871, v_i = -462.08 1/cm

C	0.000000	1.372164	-0.000112
C	0.000000	1.004030	1.212247
C	0.000000	-1.004030	1.212247
C	0.000000	-1.372164	-0.000112
C	0.000000	-0.705212	-1.223392
C	0.000000	0.705212	-1.223392
H	0.000000	1.280953	2.250422
H	0.000000	-1.280953	2.250422
H	0.000000	-1.214558	-2.182882
H	0.000000	1.214558	-2.182882

TS[43-63](¹A'): BLYP/cc-pVTZ, E = -627.88951, v_i = -420.94 1/cm

C	0.061288	-0.022641	1.429567
C	-0.195357	1.179220	1.103902
C	-0.195357	1.179220	-1.103902
C	0.061288	-0.022641	-1.429567
C	0.148745	-1.199044	-0.706951
C	0.148745	-1.199044	0.706951
F	-0.061653	-2.395455	1.303483
F	-0.061653	-2.395455	-1.303483
F	0.051869	2.423765	1.412865
F	0.051869	2.423765	-1.412865

TS[64-66](¹A'): BLYP/cc-pVTZ, E = -429.370358, v_i = -486.30 1/cm

C	0.075356	-0.693389	1.397750
C	0.075356	-1.893162	0.982088
C	0.075356	-1.893162	-0.982088
C	0.075356	-0.693389	-1.397750
C	0.038421	0.515792	-0.707171
C	0.038421	0.515792	0.707171
H	0.324345	-2.912550	1.221243
H	0.324345	-2.912550	-1.221243
F	-0.162127	1.704123	1.317773
F	-0.162127	1.704123	-1.317773

TS[65-66](¹A'): BLYP/cc-pVTZ, E = -429.355130, v_i = -416.09 1/cm

C	0.007385	0.722228	1.408031
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S22

C	-0.035749	-0.498055	1.058864
C	-0.035749	-0.498055	-1.058864
C	0.007385	0.722228	-1.408031
C	0.020868	1.927814	-0.699645
C	0.020868	1.927814	0.699645
F	0.007385	-1.755394	1.407588
F	0.007385	-1.755394	-1.407588
H	-0.021482	2.886622	1.208839
H	-0.021482	2.886622	-1.208839

TSa[75-86](¹A'): BLYP/cc-pVTZ, E = -246.9013647, v_i = -309.91 1/cm

C	-0.223004	-1.278777	0.000000
N	1.127591	-0.976095	0.000000
C	1.250324	0.341662	0.000000
C	0.000000	1.002965	0.000000
C	-1.140304	1.605527	0.000000
H	-0.542037	-2.317001	0.000000
H	2.208200	0.851019	0.000000
C	-1.114967	-0.234182	0.000000
H	-2.191594	-0.324522	0.000000

TSb[75-86](¹A'): BLYP/cc-pVTZ, E = -246.9090632, v_i = -322.54 1/cm

N	-0.284769	-1.327086	0.000000
C	1.046730	-0.952492	0.000000
C	1.253172	0.409766	0.000000
C	0.000000	1.038263	0.000000
C	-1.171564	1.570425	0.000000
H	1.816768	-1.716965	0.000000
H	2.200380	0.934490	0.000000
C	-1.102520	-0.317368	0.000000
H	-2.178667	-0.419482	0.000000

TS[(2A1)4-(2B2)4](²A'): UBLYP/cc-pVTZ, E = -230.2262514, S2 = 0.773503, v_i = -308.58 1/cm

C	-1.241676	0.974961	0.000000
C	0.000000	1.252334	0.000000
C	1.229578	0.658134	0.000000
C	1.037795	-0.750342	0.000000
C	-0.270712	-1.278659	0.000000
C	-1.370833	-0.418815	0.000000
H	2.203019	1.133934	0.000000
H	1.911150	-1.402652	0.000000
H	-0.419082	-2.356963	0.000000

TS[76(1)-76(2)](¹A'): BLYP/cc-pVTZ, E = -246.9035616, v_i = -314.77 1/cm

C	-1.325725	1.184951	0.000000
C	0.000000	1.122658	0.000000
C	1.243948	0.563716	0.000000
C	1.127446	-0.836470	0.000000
C	-0.225423	-1.217651	0.000000
H	2.174548	1.121104	0.000000
H	1.974595	-1.519556	0.000000
H	-0.553059	-2.257416	0.000000
N	-1.216794	-0.321051	0.000000

TS[80(1)-80(2)](¹A'): BLYP/cc-pVTZ, E = -246.9034335, v_i = -933.68 1/cm

N	-1.107417	0.811633	0.000000
C	-1.500587	-0.624315	0.000000
C	-0.203103	-1.254821	0.000000
C	1.070807	-0.670265	0.000000
C	1.270437	0.743749	0.000000
C	0.000000	1.255434	0.000000

S23

H	-0.263112	-2.345691	0.000000
H	1.968689	-1.291164	0.000000
H	2.221015	1.256730	0.000000

TS[76-92b](¹A'): BLYP/cc-pVTZ, E = -246.8794839, $v_i = -143.57$ 1/cm

C	-0.237712	-1.408431	0.000000
C	1.073179	-0.799668	0.000000
C	-1.468966	-0.906770	0.000000
C	1.170050	0.556892	0.000000
C	-1.159820	1.546900	0.000000
N	0.000000	1.268170	0.000000
H	-0.336829	-2.506817	0.000000
H	1.971486	-1.411399	0.000000
H	2.104960	1.107488	0.000000

TS[77-90](¹A'): BLYP/cc-pVTZ, E = -246.9300368, $v_i = -401.87$ 1/cm

N	-0.125036	-1.345612	0.000000
C	1.122030	-0.775522	0.000000
C	-1.259723	-0.891475	0.000000
C	1.204133	0.605385	0.000000
C	-1.240299	1.129252	0.000000
C	0.000000	1.317354	0.000000
H	1.998717	-1.417803	0.000000
H	2.181895	1.077878	0.000000
H	-2.262209	1.449243	0.000000

TS[79-97](¹A'): BLYP/cc-pVTZ, E = -246.9012876, $v_i = -415.40$ 1/cm

C	-0.092829	-1.391442	0.000000
C	1.129705	-1.057534	0.000000
C	1.251437	1.107727	0.000000
C	0.000000	1.262748	0.000000
N	-1.170752	0.720833	0.000000
C	-1.274740	-0.622915	0.000000
H	2.163057	-1.351441	0.000000
H	2.230290	1.549411	0.000000
H	-2.279520	-1.035308	0.000000

TS[79-88](¹A'): BLYP/cc-pVTZ, E = -246.9360327, $v_i = -460.87$ 1/cm

C	0.000000	1.322349	0.000000
N	-1.140059	0.916996	0.000000
C	-1.278790	-0.812311	0.000000
C	-0.105175	-1.345674	0.000000
C	1.142776	-0.725767	0.000000
C	1.245030	0.682876	0.000000
H	-2.329380	-1.041150	0.000000
H	2.076984	-1.284882	0.000000
H	2.209761	1.178219	0.000000

TS[80-92a](¹A'): BLYP/cc-pVTZ, E = -246.9105579, $v_i = -179.50$ 1/cm

N	-1.174792	1.354060	0.000000
C	-1.428547	-0.779387	0.000000
C	-0.207353	-1.351726	0.000000
C	1.116181	-0.788082	0.000000
C	1.247731	0.579941	0.000000
C	0.000000	1.220404	0.000000
H	-0.335588	-2.443191	0.000000
H	1.997012	-1.429480	0.000000
H	2.194055	1.107355	0.000000

TS[88-92a](¹A'): BLYP/cc-pVTZ, E = -246.9151854, $v_i = -69.80$ 1/cm

N	2.338225	0.141658	0.000000
C	-0.815794	-2.082594	0.000000

S24

C	-1.282597	-0.872256	0.000000
C	-1.172476	0.562727	0.000000
C	0.000000	1.246970	0.000000
C	1.279956	0.632677	0.000000
H	-2.304739	-1.382308	0.000000
H	-2.099313	1.130714	0.000000
H	-0.018052	2.334840	0.000000

TS[90-92b](¹A'): BLYP/cc-pVTZ, E = -246.8806712, $\nu_i = -115.59$ 1/cm

C	-1.187763	-0.923808	0.000000
C	-1.143921	0.510875	0.000000
C	-0.763621	-2.143651	0.000000
C	0.000000	1.235053	0.000000
C	2.349889	0.223518	0.000000
N	1.253255	0.673889	0.000000
H	-2.189188	-1.503167	0.000000
H	-2.085401	1.052207	0.000000
H	-0.025707	2.321814	0.000000