

Supporting Information

I. MP2/6-31G* optimized structure and raw energies of H₂ interacting with various organic linkers (H₂-BDC-X) (X= H, F, CH₃, NH₂, OH) in the perpendicular configuration.

(i) H₂-BDC-H

H	0.0025177215539744	-0.0036640363512806	-3.0080288963880735
H	-0.0000618516540394	-0.0134788671483413	-3.7460629771660767
C	-1.3928899130306891	0.0342012021426889	0.0354533644145998
C	1.3926068943135324	0.0342054392111187	0.0351574598643629
C	-0.6964347991597355	-1.1820010034623811	0.0359379538819825
C	-0.6950669289341037	1.2496329642623045	0.0356470091982215
C	0.6947791492612586	1.2496359835210626	0.0355045223114502
C	0.6961528873549524	-1.1820000813211586	0.0357917524879914
C	2.8773139203379507	0.0909570565078902	0.0353840677750806
O	3.5369344191143473	1.1190551470309094	0.0377905418880531
O	3.4471035923007638	-1.1443150405483220	0.0329602994942145
C	-2.8775963263177609	0.0909494235362621	0.0359512788510391
O	-3.5372196808103635	1.1190458458748014	0.0383293864223661
O	-3.4473866445023740	-1.1443230262305066	0.0336043680374117
H	1.2580999942187676	2.1785031567066504	0.0356702740917372
H	-1.2583909222074661	2.1784978818783260	0.0359152170562059
H	-1.2450156975767586	-2.1185419744499794	0.0362962367211336
H	1.2447363112118468	-2.1185399754774461	0.0360413916739106
H	4.4133571930235540	-0.9819181253443258	0.0330505444468014
H	-4.4136401778092056	-0.9819261011499419	0.0337881261293878

MP2/6-31G* Energy = -608.796834548 a.u.

RIMP2/cc-pVTZ//MP2/6-31G* Energy = -609.4980731760 a.u.

RIMP2/cc-pVQZ//MP2/6-31G* Energy = -609.6949409886 a.u.

(ii) H₂-BDC-CH₃

H	0.1217920635865324	0.2122621903831436	-2.9344623391253011
H	0.1176118842780817	0.2100343434376034	-3.6726687504719742
C	-1.2652048867284151	0.3008651518603008	0.0754450756328358
C	1.5249721834398722	0.1572246903796974	0.0768245174826046
C	-0.6470825195053816	-0.9720167387980102	0.0584545340689183
C	-0.4853648211100970	1.4699983372805987	0.0934675321883524
C	0.9003458192166819	1.4086882347201286	0.0933357591872679
C	0.7535704744579019	-1.0089355045937918	0.0609156016841713
C	3.0092493408923899	0.1199230324781661	0.0774222880007638
O	3.7317953402175599	1.1051135740961275	0.0912503098609325
O	3.5033218843231100	-1.1480344264792006	0.0608895078203392
C	-2.7367980718967999	0.5498155476253495	0.0768916542928568
O	-3.2440201176072208	1.6615019369647948	0.1195703844607724
O	-3.4974540648931436	-0.5756426000792281	0.0229492508740333
H	1.5080757840260721	2.3088549094130690	0.1048991170794331
H	-0.9992916306182672	2.4264049057313022	0.1069544157165914
H	1.2561612724342681	-1.9719576069822053	0.0490143127934398
H	4.4775323300038137	-1.0432192340662252	0.0624977048308128
H	-4.4221200300408841	-0.2478245825733991	0.0291671284398103
C	-1.3858583264916819	-2.2877093016362613	0.0388435047515901
H	-2.0168666515142086	-2.3810541076523108	-0.8472454458143912
H	-0.6633125468368108	-3.1079347477309001	0.0400881031962849

H -2.0375943570788317 -2.3966503415341536 0.9079988540770642

MP2/6-31G* Energy = -647.964164671 a.u.

RIMP2/cc-pVTZ//MP2/6-31G* Energy = -648.7214576183 a.u.

RIMP2/cc-pVQZ//MP2/6-31G* Energy = -648.9312453221 a.u.

(iii) H₂-BDC-F

H 0.1248147962098247 0.1815928764880992 -2.9412486546560741
H 0.1210475574007792 0.1740796187936470 -3.6792437108053662
C -1.2885961130405186 0.2610708666877760 0.0717962164692190
C 1.5187569463763162 0.1562188737926227 0.0737877505174653
C -0.6066716166252235 -0.9633986731843343 0.0641412323905592
C -0.5223711100769979 1.4387507495871410 0.0817229500429628
C 0.8650312270350814 1.3958423529930943 0.0829847207542046
C 0.7814887845399489 -1.0309774918661898 0.0651345989043504
C 3.0050821838754493 0.1502275397153095 0.0748532573489869
O 3.7035295788939480 1.1519043573457741 0.0847851175421889
O 3.5196998171228588 -1.1074420578289366 0.0636040760334215
C -2.7689857440744325 0.4274823923027442 0.0703119276423628
O -3.3212009183959763 1.5177795978159248 0.0894529014944489
O -3.4531407741596150 -0.7390062434807523 0.0444228154752839
H 1.4575968565794009 2.3055878668314858 0.0898916001276663
H -1.0541271677182187 2.3856256761082024 0.0883526857323545
H 1.2654244598197499 -2.0016858118879228 0.0584198004405035
H 4.4926839146562028 -0.9909017819678061 0.0650018884277161
H -4.3979522920058187 -0.4757648545609002 0.0453795245361439
F -1.2798024437534465 -2.1318512837969461 0.0571510346904546

MP2/6-31G* Energy = -707.809178016 a.u.

RIMP2/cc-pVTZ//MP2/6-31G* Energy = -708.6204158138 a.u.

RIMP2/cc-pVQZ//MP2/6-31G* Energy = -708.8488309972 a.u.

(iv) H₂-BDC-NH₂

H -0.1142409883792767 -0.2213757231093219 -3.6751765624890527
H -0.1244253819701761 -0.2443847980758900 -2.9373737391990700
C 1.2807581940713870 -0.2198485514135803 0.0805401289597051
C -1.5112306017131203 -0.1034324611356245 0.1004372166515863
C 0.6399288925388947 1.0479753318480018 0.0927398239414535
C 0.5098781187783664 -1.3972424796127603 0.0995433502850654
C -0.8752618493478267 -1.3557474542960199 0.0945120104672122
C -0.7665915503663898 1.0718014520333285 0.0805877124482807
C 2.7521955766029249 -0.3087444372192329 0.1384134726382198
O 3.5292663846856689 0.6362139863297884 0.2643354799223183
O 3.2141040867165986 -1.5834592588773999 0.0407382570142237
C -2.9894504332017666 0.0324121179670542 0.1055783413496102
O -3.5986819311735343 1.0926975788895434 0.1160138199437063
O -3.6234297121468289 -1.1712426395711408 0.0993550163222156
N 1.3341215400268349 2.2337284977074146 0.0068883516968498
H -1.2939743964221226 2.0234750499682415 0.0760887147025704
H -1.4598494891930653 -2.2690480266048563 0.1086674460037413
H 1.0233270953731468 -2.3531051217434968 0.1005944009436918
H 0.8343118226851218 3.0598274363661924 0.3100365148525285
H 2.3154855051820600 2.1933435754099131 0.2580656305330101
H 4.1887050501606113 -1.5031037722981484 0.1013997465178162

H -4.5794154713189990 -0.9565438089543873 0.1030441438221127

MP2/6-31G* Energy = -663.995354148 a.u.

RIMP2/cc-pVTZ//MP2/6-31G* Energy = -664.7690460512 a.u.

RIMP2/cc-pVQZ//MP2/6-31G* Energy = -664.9853716097 a.u.

(v) H₂-BDC-OH

H 0.1322306373625874 0.2010764421436696 -2.9378443304940851
H 0.1290878064394006 0.1981748522694187 -3.6759987727813299
C -1.2680699398296167 0.2827270718816466 0.0724347535659002
C 1.5261670154246096 0.1421318934529406 0.0756555146487265
C -0.6255852246927559 -0.9768462745552430 0.0563693066058779
C -0.4872401214962507 1.4544584921889674 0.0900234989706672
C 0.8953211882433814 1.3968689240002445 0.0917814273428427
C 0.7749008014228999 -1.0305767978820271 0.0590782817801781
C 3.0114155437576926 0.1135978125606480 0.0777823571556048
O 3.7260275310221265 1.1048217025491189 0.0932836162568424
O 3.5121274645553395 -1.1503479387076201 0.0606431996729792
C -2.7343243052044550 0.4847664604507005 0.0722000773537366
O -3.3060524652150485 1.5601203725866049 0.0908048365379427
O -3.4437456500680721 -0.6945585230446559 0.0476144276077028
H 1.5012679804311821 2.2973595739458177 0.1040981920036722
H -1.0071299406498633 2.4081859438726902 0.1022148233604495
H 1.2509937542911631 -2.0055518350250252 0.0464535327724721
H 4.4858861259443223 -1.0416491221207620 0.0633790432301941
H -4.3904164167022879 -0.4393508458902372 0.0495536551697858
O -1.2528464310153724 -2.1811008645420742 0.0401518408423218
H -2.2198296786893779 -2.0331525122668270 0.0363725150607728

MP2/6-31G* Energy = -683.834602589 a.u.

RIMP2/cc-pVTZ//MP2/6-31G* Energy = -684.6264171503 a.u.

RIMP2/cc-pVQZ//MP2/6-31G* Energy = -684.8483431291 a.u.

2. MP2/6-31G** optimized geometry and raw energies of the ligand-H₂ complexes.

(i) NO⁺-H₂

H 2.572353 -.152106 -.020008
H 2.497335 .579249 .013693
N -.203467 -.537934 -.000440
O -.763747 .412634 .004663

MP2/6-31G** Energy = -130.401554997 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -130.0853498903 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -113.155076166 a.u.

CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -130.555686099 a.u.

(ii) CO-H₂

H 2.840149 .042326 -.002134
H 3.573698 .065802 .001697
C -1.113366 .051129 .000002
O .033293 -.051863 .000053

MP2/6-31G** Energy = -114.179442908 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -113.9094451381 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -114.3003795385 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -113.155076166 a.u.

(iii) OC-H₂

C	-0.0641386311924628	0.0024828385444003	0.0000000000000000
O	-1.2150228338687665	-0.0012932748647740	0.0000000000000000
H	3.6722199254474601	-0.0022955445089368	0.0000000000000000
H	2.9379723780540496	-0.0007640969631703	0.0000000000000000

MP2/6-31G** Energy = -114.179611961 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -113.9092491203 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -114.3003965571 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -113.155100939 a.u.

(iv) CN⁻-H₂

H	3.158717	-.003255	.000000
H	2.411658	-.002146	.000000
C	-1.075082	-.002051	.000000
N	.125731	.002530	.000000

MP2/6-31G** Energy = -93.727997599 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -93.4653088421 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -93.8438072157 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -92.693522689 a.u.

(v) NC⁻-H₂

C	0.0917316933293856	0.0011825361352949	0.0000000000000000
N	-1.1072755799076608	-0.0008763046743052	0.0000000000000000
H	3.2264369185158626	-0.0030661714373550	0.0000000000000000
H	2.4764441296916777	-0.0017873126720473	0.0000000000000000

MP2/6-31G** Energy = -93.729610810 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -93.4649159663 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -93.8443644222 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -93.872045066 a.u.

(vi) Cp⁻-H₂

H	.063881	-.011350	3.114844
H	.063248	-.011029	2.373963
C	.084826	-1.197986	-.160144
C	-1.116206	-.453969	-.146175
C	-.779769	.918253	-.147000
C	.629260	1.022428	-.161964
C	1.163713	-.285531	-.169984
H	-2.120514	-.864387	-.134320
H	.164744	-2.280040	-.161784
H	2.217444	-.543935	-.180071
H	1.200542	1.944845	-.164302
H	-1.480292	1.746727	-.136736

MP2/6-31G** Energy = -194.036241291 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -193.3950831902 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -194.3358504309 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -193.149004668 a.u.

(vii) $F^-(H_2)_n$ (n = 1-4)
 $F^-(H_2)$

F 0.0930897568895016 0.1054436156858341 0.0000000000000000
H -1.3402325382326932 -0.0159062005682337 0.0000000000000000
H -2.1889574191966634 -0.0877627013129825 0.0000000000000000

MP2/6-31G** Energy = -100.719006000 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -100.5705876527 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -100.8943914143 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -100.906957810 a.u.

$F^-(H_2)_2$

F -0.0199730117986961 0.9841283480789196 0.0153880876895511
H -1.3618690934017994 -0.0101351949907466 0.0168346023421873
H -1.9978529430687382 -0.4707252281325854 0.0174875023877294
H 1.2844760372442652 -0.0587101536256329 0.0206246951342187
H 1.9031552609823279 -0.5423055910173482 0.0230743494942089

MP2/6-31G** Energy = -101.898308125 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -101.7150054734 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -102.0748135601 a.u.

$F^-(H_2)_3$

F -0.0591504055813054 -0.0044260040547462 0.6972013153798661
H -0.9192907976669358 1.3539655910744066 -0.0250972604991196
H -1.2962616871201433 1.9495497568103535 -0.3333082657290393
H -0.8291423938967847 -1.4216807459163603 -0.0137823578072352
H -1.1665344377777189 -2.0429815053794966 -0.3170351871750879
H 1.5289824389367064 0.0438409121234440 -0.0657013634399562
H 2.2254279800087171 0.0650288544587119 -0.3917990844389228

MP2/6-31G** Energy = -103.074251320 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -102.8575210600 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -103.2533262556 a.u.

$F^-(H_2)_4$

F 0.0578053744514562 0.0001796534545371 0.0192413192912813
H 0.9378999899691580 -0.3104786987076550 -1.5435046602876397
H 1.3060142503850438 -0.4404150959643310 -2.1971404918023874
H 0.4718952669163037 -1.3043966978567820 1.2191976765815862
H 0.6450903089986009 -1.8500531141272911 1.7210877386362744
H 0.5574993542974462 1.6182923927493675 0.6865496547125904
H 0.7664979448855603 2.2950878052374128 0.9656529848513316
H -1.7371915781551988 -0.0023373777525736 -0.2828697756461195
H -2.4879657736242375 -0.0033966118287028 -0.4092453019443286

MP2/6-31G** Energy = -104.247695276 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -103.9990846057 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -104.4302935028 a.u.

(viii) $\text{SO}_4^{2-}-(\text{H}_2)_n$ (n = 1-8)

$\text{SO}_4^{2-}-(\text{H}_2)$

O	-1.1172587984413915	-1.0027915320561496	0.7324439401841902
S	-0.4607986770336007	0.1941576573348237	0.0769508784304510
O	-0.9005878799303887	0.2951125586621370	-1.3686525632437718
O	-0.8349930807427526	1.4596796076173524	0.8200012239585733
O	1.0594187087114886	0.0286127910055280	0.1316602766266288
H	2.7099324462879135	-1.9184255276118172	-0.8890285697930883
H	2.1930726707532289	-1.4205551354399764	-0.6377592373045462

MP2/6-31G** Energy = -698.837554185 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -698.1179587847 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -699.3877017563 a.u.

CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -699.431614430 a.u.

$\text{SO}_4^{2-}-(\text{H}_2)_2$

O	-0.9476049193417084	-1.1899781733621895	0.2680711069312413
S	-0.0463230647744156	0.0356741499505746	0.1578727334208088
O	0.0609898546380287	0.4588150242902635	-1.2885602442970165
O	-0.6127959857247637	1.1605655297418489	0.9925738831720973
O	1.3350642400571540	-0.3325335646162800	0.6897242472948889
H	3.2513406243651146	-2.1180384516175037	-0.2156122905690824
H	2.6831175209229463	-1.6528187420650045	-0.0286498952318220
H	-2.9033496110485029	-1.3732152738600159	-0.2022829040853829
H	-3.6279318811110914	-1.5418795204216058	-0.3467773388403642

MP2/6-31G** Energy = -700.007069897 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -699.2583621599 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -700.5637265831 a.u.

$\text{SO}_4^{2-}-(\text{H}_2)_3$

O	-0.1563684294541868	1.6498049347817381	-0.6246399824109177
S	-0.1956058365838179	0.1681514922494286	-0.2822737479553037
O	-0.0929677399873953	-0.0206716149675125	1.2101477057887815
O	-1.5014129119653414	-0.4209692864296349	-0.7940413282219307
O	0.9644605908257231	-0.5285208019773446	-0.9772576204487079
H	3.7285587638011641	-0.2078337569008000	-0.7494608002733637
H	2.9735101061015818	-0.2395704231246835	-0.7589906195828930
H	-1.3782728902331454	3.1614474320764341	-0.0007036584820959
H	-1.7714646739679423	3.7834900809668417	0.1715048503461989
H	-2.2193509230336379	-2.3253437042661189	-0.6352528723864034
H	-2.5682519916405289	-2.9957384874082349	-0.6290981329928941

MP2/6-31G** Energy = -701.175898675 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -700.3984915485 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -701.7390591192 a.u.

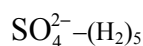
$\text{SO}_4^{2-}-(\text{H}_2)_4$

O	-0.4731122673863490	-1.0425164231736830	-0.5610386034977251
S	0.2284993012821431	0.3015744235364444	-0.5001840449901118
O	-0.5565176640186215	1.3306538434889141	-1.2926273519161764
O	0.3379294769577353	0.7596925124407929	0.9422976352230853
O	1.6133155624534463	0.1698000404557624	-1.1068961910245037
H	3.5818304010395789	-1.8277974661712360	-0.9295422981161217
H	3.0102720760265429	-1.3363076235052873	-0.9282951271285405
H	-2.3622426524979701	-1.6236104067824886	0.0409164003693848
H	-3.0257511329243409	-1.9296413630407223	0.2249011670804962
H	1.2800182237398663	-0.0878903762311592	2.5740158239024278
H	1.5902416996549529	-0.3143835272884707	3.2222660009338902
H	-2.2662138851073386	2.3743852244115042	-0.8035833982088634
H	-2.8809305196327211	2.8028212706418030	-0.7210950685959597

MP2/6-31G** Energy = -702.343806909 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -701.5382464461 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -702.9134948660 a.u.

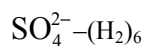


O	0.3524849468599356	-0.2736512224495142	-1.0047008047079820
S	0.0087825333042741	-0.0364739736166815	0.4638774245282842
O	1.1854114009074757	-0.4305243958777251	1.3325270323556646
O	-0.3043919337507716	1.4307979612693207	0.6676583271861178
O	-1.1880352317863514	-0.8864755345376891	0.8359776355911888
H	-3.8027746846991977	-1.1575252025973677	-0.2078992704401394
H	-3.0948637276867603	-1.0335496359604006	0.0139860132898070
H	1.5763638972907981	0.8789346708602447	-2.2557083068075032
H	1.9945029268834911	1.2234073400145185	-2.7769796843260544
H	-1.7914141761248072	2.6656766258644131	-0.1106316154579238
H	-2.2864310489715858	3.1863263731476339	-0.3328786230534507
H	2.9724649212194616	0.5559837858537198	1.7245003137095447
H	3.6419430955841317	0.8316239047224263	1.9295339108420062
H	0.7822103551806610	-2.7143215180120630	-2.3942832617777001
H	0.6557737804570420	-2.1081274607865645	-1.9674281604950492

MP2/6-31G** Energy = -703.511323682 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -702.6774139378 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -704.0875472647 a.u.



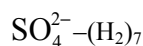
O	-0.6916400004009658	-1.1957531945830027	0.1538061889946524
S	0.0849738955131075	0.1102082396762592	0.0451785007751200
O	-0.6232725263837525	1.0574705783558509	-0.8963526735753420
O	0.2044388923364952	0.7387170340047668	1.4145629089178731
O	1.4691060735038513	-0.1970059306791876	-0.5119181485609711
H	3.3589814104028450	-2.2273744493037828	0.1558637630825396
H	2.8170036383253101	-1.7224262378966877	0.0337503264572853
H	-2.4312804869699787	-1.5741477666264052	1.2878317629878169
H	-3.0461630329265819	-1.8022526147837277	1.6532322656751353
H	1.0568894654097949	0.0634695989848179	3.2114251149850519
H	1.3340305057570521	-0.0894226399246589	3.8922539255670348
H	-2.3197053343664278	2.2527127226078005	-0.6038803019812401
H	-2.9139604756509270	2.7122271611931619	-0.5945504076966138

H -1.2785984694943646 -3.1589897258881585 -1.8359137827079663
H -1.0879871696169183 -2.6069957359809788 -1.3639248811909024
H 2.8281107196286932 1.1671413755464553 -1.3586340123171876
H 3.3744497320576285 1.5764161470212970 -1.6723318097031050

MP2/6-31G** Energy = -704.678533403 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -703.8164331154 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -705.2613434509 a.u.

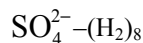


O -0.4073938512389479 1.2078570436237737 -0.7001309274444005
S -0.0217617277507073 -0.0824129289153990 0.0049736528365124
O -0.7886474518151295 -0.2265238794969231 1.2966439893439885
O -0.3360011075920716 -1.2529384057990107 -0.9125942151999065
O 1.4673971092987712 -0.0504436284845267 0.3086705579878903
H 3.7246485116723229 0.6940780143693996 -1.2935088958858136
H 3.0913945239192859 0.5152869491437470 -0.9341522016947965
H -2.1449846319615427 1.6067544324170857 -1.8564371890857398
H -2.7215396651257606 1.8416191825543791 -2.2741328529882119
H 0.1232569459662193 -1.5167441939519997 -2.9718061051029996
H 0.2404705109228737 -1.6989825456381276 -3.6893754865315045
H -2.8586564026851904 -0.3772930652304960 1.6915343209714460
H -3.5681209468574893 -0.4350831221246718 1.9277348879758724
H 0.0393730543373935 3.9298587016548545 0.0815215952948474
H -0.0422264455865458 3.1986495027439656 -0.0640293190918444
H 2.4973497833974894 -1.0711563304587857 1.8553211958628013
H 2.9462673023499324 -1.3883207053850151 2.3656095901827610
H -0.4786438113120193 -3.3130761332257181 -0.4150592174491437
H -0.5481473602225030 -4.0553995958536131 -0.3356273013772663

MP2/6-31G** Energy = -705.845190550 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -704.9552487858 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -706.4346253599 a.u.



O 0.5609371896571819 -0.9492344895215161 -1.2254545827008083
S 0.1487620988932662 0.0915618025340538 -0.2012215881595844
O 1.2509873641533864 0.2844223448027385 0.8235504447267469
O -0.1076501578482517 1.4092958648942497 -0.9083183934186592
O -1.1093019279145917 -0.3780744421253840 0.5050927071077254
H -3.5006957871022442 -1.6039215661478523 -0.5342446539138815
H -2.8533201755059658 -1.2852236512993485 -0.3339121690907940
H 1.9409554111947409 -0.7559858474144405 -2.8473383053417103
H 2.4048919933243331 -0.7837868136915570 -3.4344794828341585
H -1.2286163487977382 1.7807913843657066 -2.6908012562015733
H -1.5991106820399765 2.0059649394211769 -3.3013499572003839
H 3.1228613725770460 1.2922038982455704 0.6096270521927861
H 3.7964287406996307 1.6189444685390391 0.6287487819076525
H 0.8544657364035992 -3.8083649833198923 -1.0032467790521662
H 0.7576267243998988 -3.0659541537400621 -0.9912794550219767
H -2.0141428405288675 0.3817595730798957 2.2863849197884787

H	-2.4001055319151123	0.5794506503380935	2.8968892148437866
H	-0.3108470570454599	3.3642698462400911	-0.0689502284759469
H	-0.3964885679080475	4.0803150368188890	0.1328634417925475
H	2.1044718976942649	-1.3827172840897324	3.0136293932633627
H	1.8311263679335703	-1.0002265969725259	2.4307561103831525

MP2/6-31G** Energy = -707.011475108 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -706.0937859619 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -707.6075057907 a.u.

3. MP2/6-31G** optimized geometries and raw energies of H₂-metal ions/complexes.

Li⁺-(H₂)

H	1.4284932844844465	-0.3721809568477610	0.0000000000000000
H	1.4296750057798706	0.3692429270246443	0.0000000000000000
Li	-0.6597707243803709	0.0019411487121693	0.0000000000000000

MP2/6-31G** Energy = -8.401061339 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -8.3785049255 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -8.4214213192 a.u.

CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -8.431168391 a.u.

Li⁺-(H₂)₂

H	2.0582508868442062	-0.2654290616437625	0.3558662506366110
H	2.0752131195701939	0.2419362037607024	-0.1842004250333665
H	-2.0966363835059649	-0.2530914100394224	-0.2120544210732609
H	-2.0977005819372136	0.2685384802747960	0.3144781428331130
Li	-0.0155432370524526	0.0131679442287192	0.0493578999975619

MP2/6-31G** Energy = -9.566123671 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -9.5202578786 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -9.5953593318 a.u.

CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -9.612776240 a.u.

Li⁺-(H₂)₃

Li	0.0206778558795746	-0.0112886421520449	-0.0081391679810008
H	2.1358960293267923	0.1247392601469323	0.1440209902459408
H	2.0688474521905902	-0.5655450828049540	-0.1166247147333727
H	-1.5574046687782708	-1.4313128280313814	-0.0976287402324174
H	-0.9955944382783857	-1.8756446797406163	0.0916849930235993
H	-1.0850593661090699	1.7841683483572675	0.2732630591962533
H	-0.6287890402225723	1.9974437067960173	-0.2700966385640246

MP2/6-31G** Energy = -10.730669404 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -10.6610156053 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -10.7686117186 a.u.

CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -10.793750195 a.u.

Li⁺-(H₂)₄

H	-1.1459325059627297	-1.5678598302447226	0.8643686467662486
H	-1.6585366506915469	-1.2807643852329467	0.4136551187702184

H	-0.1323463041420314	1.9992988829636729	0.6414704680865276
H	-0.8285208173124020	1.7784838519482540	0.7637577699656902
H	2.0174097795763468	-0.6147489158662834	0.2534760153136388
H	1.8266245687399649	-0.4499674681547089	0.9497553653803115
Li	-0.0062863620665263	-0.0139114685120562	-0.0504152116364740
H	-0.0480579476084826	0.3794963367673957	-2.1462392294745452
H	-0.0673056810035322	-0.3607132283576892	-2.1540399738316154

MP2/6-31G** Energy = -11.894924512 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -11.8007106391 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -11.9411642841 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -11.974048306 a.u.

Li⁺-(H₂)₅

Li	-0.0020546649827033	-0.0000798148006075	0.1245832014848392
H	2.0633476088066440	-0.0450544118242743	0.8555284151445556
H	2.1796397872242630	-0.0199177406644055	0.1256201968482117
H	0.0188588495199575	0.3718017180699310	-1.9941948240996124
H	0.0061160668814034	-0.3680338374238888	-1.9947539315252323
H	-2.1840814540311069	0.0199036260571142	0.1100921787965888
H	-2.0721095091598136	0.0436765888289386	0.8407331675491122
H	0.4004051791097800	2.1237000046012033	0.4353158905526350
H	-0.3382072719911535	2.1389713118169933	0.4087766004008438
H	0.3352088644905196	-2.1404933975368041	0.4018885470118396
H	-0.4030215038184704	-2.1243462588423490	0.4372700954785745

MP2/6-31G** Energy = -13.056885963 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -12.9369282882 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -13.1109366293 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -13.151627160 a.u.

Li⁺-(H₂)₆

H	1.9038778041911841	0.5824684590726020	-0.8994232488592080
H	1.4749852263967695	1.1291441846269177	-1.1511388953323349
H	-1.2408000369300791	1.7350394466536074	-0.5440854574556233
H	-1.3554063219247932	1.3106618746982641	-1.1381825938519374
H	1.1948312514664452	-1.7550008771313261	0.5721140461166158
H	1.3573298790469979	-1.3059023899257216	1.1361074410499059
Li	-0.0130080296234266	-0.0047047966032786	0.0065357367431066
H	0.0922795997680058	1.1225575319210392	1.8966459099777060
H	0.6572981386307003	1.4329649247088458	1.5353106073643350
H	-0.1249955437008342	-1.1284595317965196	-1.8851658905705713
H	-0.6868647686151926	-1.4411630689596127	-1.5208585760691564
H	-1.4934302773853061	-1.1163034911659129	1.1972930489707478
H	-1.9375912759485681	-0.6137505001904608	0.8868758814859742

MP2/6-31G** Energy = -14.219326596 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -14.0735408110 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -14.2812231839 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -14.329724579 a.u.

Na⁺-(H₂)

H	1.8948750043143427	-0.3693128165312095	0.0000000000000000
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H 1.8948567451968017 0.3693204227369358 0.0000000000000000
Na -0.5761045908302338 -0.0000027982207036 0.0000000000000000

MP2/6-31G** Energy = -162.822451789 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -162.8138357227 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -162.8555845519 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -162.864120797 a.u.

Na⁺-(H₂)₂

Na 0.0000400000000000 0.0016980000000000 0.0035490000000000
H 2.4730360000000000 0.2711009999999999 0.2355970000000000
H 2.4692189999999998 -0.2806919999999998 -0.2552700000000000
H -2.4717169999999999 -0.2783730000000000 0.2380550000000000
H -2.4709810000000001 0.2692910000000000 -0.2574200000000000

MP2/6-31G** Energy = -163.984067740 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -163.9515190215 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -164.0261914346 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -164.042481580 a.u.

Na⁺-(H₂)₃

H 1.7096402320150612 -1.8230224456326278 0.0430466167594290
H 1.1065218610413627 -2.2422367165706256 -0.0328738253211153
H -2.4995720307572671 0.1839680619992569 -0.0317709297960847
H -2.4462568069658310 -0.5487190142127508 0.0429702060182065
H 0.7558041962269456 2.3818146263143647 0.0406108628078843
H 1.4157146711597854 2.0581852311247641 -0.0303681478997925
Na -0.0050718273431261 -0.0012159511820747 -0.0037395075861670

MP2/6-31G** Energy = -165.145607569 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -165.0888677136 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -165.1955931793 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -165.219576607 a.u.

Na⁺-(H₂)₄

H 1.3894151761780456 -1.0456604333511583 1.8029083237465326
H 1.7866329286347291 -1.2629405208577338 1.2197607128146986
H -1.6254554333166280 -1.4102569933906015 -1.2809291498507418
H -1.1154943464311537 -1.9271613159492680 -1.1475022732860820
H -1.3457245143009968 1.7582294929791777 1.1675956941679904
H -1.6733381126702764 1.1624364113989925 1.4552759602501513
Na 0.0000002946158682 -0.0012229085416824 0.0003672407283560
H 1.0735945675018213 1.2518264255630955 -1.8828830155888088
H 1.5102206717665578 1.4842409469744184 -1.3347959494296697

MP2/6-31G** Energy = -166.307067490 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -166.2259575653 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -166.3654270891 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -166.397155147 a.u.

Na⁺-(H₂)₅

Na -0.0016594963426634 -0.0001842895118149 0.1125149164211347

H	2.4030606937346812	-0.0504635010493579	0.8872655225774236
H	2.5166646600182734	-0.0250816002958562	0.1584974513934208
H	0.0219375814477616	0.3710613501040124	-2.3709577825650792
H	0.0092199655830533	-0.3669190000771366	-2.3716229842699805
H	-2.5201944814537680	0.0247817103255452	0.1397601631710749
H	-2.4115472808231395	0.0487885503493980	0.8693339951690893
H	0.4051965220727755	2.4620160437582812	0.4653830303937003
H	-0.3321420121065328	2.4768961308231683	0.4397171448717817
H	0.3296332788111845	-2.4780720278706241	0.4325245673258309
H	-0.4073562952701485	-2.4624241766362842	0.4664368560981418

MP2/6-31G** Energy = -167.468146363 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -167.3622635691 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -167.5355862161 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -167.575152401 a.u.

Na⁺-(H₂)₆

H	0.2834568345294555	2.0849953707559172	-1.3992402397770132
H	0.6381065663582592	2.3125108978425613	-0.7935648669690062
H	1.3896057872837797	0.6900589796881538	1.9937930728023789
H	0.7413342287279140	0.9641771472458091	2.2151182733050558
H	-1.3939693397266484	-0.7146390151134229	-1.9831115667171013
H	-0.7345146902153330	-0.9341604045196608	-2.2307294799182897
Na	-0.0006090024447863	-0.0001308266878647	-0.0001119803974072
H	2.1426736506099902	-1.1823890725180455	-0.6288231118633604
H	2.2888512665316116	-0.5257533288939189	-0.9318790356677065
H	-2.1417634105887728	1.1816842529748703	0.6363704653281624
H	-2.2888773450152562	0.5232363326318261	0.9350150362732617
H	-0.6041637045411566	-2.3268273957746688	0.7787933013369239
H	-0.3154322572350406	-2.0742826282909861	1.4090626781173519

MP2/6-31G** Energy = -168.629301234 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -168.4984640777 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -168.7056352439 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -168.753036593 a.u.

Mg²⁺-(H₂)

H	1.7722902577981321	-0.3820096479472829	0.0000000000000000
H	1.7722690067753555	0.3820166230688252	0.0000000000000000
Mg	-0.2620686667778879	-0.0000021294717892	0.0000000000000000

MP2/6-31G** Energy = -200.005192521 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -199.9969184700 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -200.0436745132 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -200.052226621 a.u.

Mg²⁺-(H₂)₂

H	2.0340429958386408	-0.2999694466255644	-0.2620334560257719
H	2.0399218839868540	0.2717855512217771	0.2415667090333620
H	-2.0369831854723026	0.2501934035185809	-0.2846404596969565
H	-2.0357659474300811	-0.2764677735971470	0.2659882699354126
Mg	0.0002969337219431	0.0005559005234896	-0.0010443222904362

MP2/6-31G** Energy = -201.192759576 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -201.1618905487 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -201.2424780438 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -201.258962646 a.u.

Mg²⁺-(H₂)₃

H	1.4773015002070844	-1.4717463325354041	0.0094210492699526
H	0.8537559147069653	-1.9038462741837205	0.0001802972246543
H	-2.0739125899824753	0.2270872439930580	0.0026284237223153
H	-2.0168787280771459	-0.5294802799460608	0.0060045588117091
H	0.5582014695508593	2.0100497843447069	0.0093627571386394
H	1.2398377315940747	1.6771062774980365	-0.0012078340102816
Mg	-0.0000945279831596	-0.0000558775569011	0.0025700326609772

MP2/6-31G** Energy = -202.375512367 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -202.3222011650 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -202.4358770864 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -202.460232858 a.u.

Mg²⁺-(H₂)₄

H	1.1179897717224871	-0.8510809526864729	1.5592285502781047
H	1.5243052884361168	-1.0732784871198511	0.9616457769530700
H	-1.3988193092012398	-1.1247286593729162	-1.0842262184739426
H	-0.8796498204599581	-1.6555284776126074	-0.9418406038834166
H	-1.0881857569929829	1.5232257864981058	0.9479067312256902
H	-1.4235772141787344	0.9122458580123436	1.2408308327005417
Mg	0.0000216518632323	-0.0005027865847788	0.0006416569186170
H	0.8508864161292053	1.0200635339129513	-1.6229734893570480
H	1.2968735096835300	1.2595023895410573	-1.0614248009133833

MP2/6-31G** Energy = -203.555984212 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -203.4788692596 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -203.6265947206 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -203.658849626 a.u.

Mg²⁺-(H₂)₅

Mg	-0.0010581267390841	-0.0003515275972395	0.0475927258103080
H	1.9301184731197565	-0.0260838073241119	0.9517779516724825
H	2.1165490432942757	-0.0344438695899631	0.2223540318746880
H	0.0305479779476223	0.3782625983335673	-2.0315953763760013
H	-0.0141817816705723	-0.3735612538663534	-2.0332999135854943
H	-2.1189402454935302	0.0332559085152499	0.2031519506155707
H	-1.9396420305170619	0.0248633045294412	0.9344116374413468
H	0.4092564110975007	2.0844280261031671	0.2408442101328020
H	-0.3417115159933872	2.0993855020671868	0.2091144279147966
H	0.3467565155444993	-2.0985927046279906	0.2073302773381726
H	-0.4042317944255934	-2.0867427408615211	0.2386137537397871

MP2/6-31G** Energy = -204.730657394 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -204.6273297402 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -204.8106369479 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -204.850845110 a.u.

Mg²⁺-(H₂)₆

H	0.2090873533428773	1.7414200992817424	-1.2345830577483179
H	0.5689446477460676	1.9732451970790161	-0.6181697843438806
H	1.2295279750833235	0.5590679632308885	1.6653813086598790
H	0.5701166822574056	0.8375749549207029	1.8907911184963722
H	-1.2339481848385914	-0.5841727714299573	-1.6541199190841049
H	-0.5633433029637313	-0.8081662985469819	-1.9057952280565855
Mg	-0.0004050506241637	-0.0001067289183299	-0.0000757450000888
H	1.7976150254838685	-1.0555309463063245	-0.5051117364345292
H	1.9459587657970405	-0.3878521648859170	-0.8139711868754560
H	-1.7965547739188639	1.0550301106160249	0.5115652791166130
H	-1.9457835091847979	0.3854750985005457	0.8159518555365904
H	-0.5351821149566000	-1.9870911464120875	0.6039338204099723
H	-0.2410804196106160	-1.7304953672903383	1.2449333313464854

MP2/6-31G** Energy = -205.905339770 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -205.7757874552 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -205.9947997560 a.u.

CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -206.042963721 a.u.

Al³⁺-(H₂)

H	1.6981245607301407	-0.4391738592448241	0.0000000000000000
H	1.6981055854681735	0.4391783886103015	0.0000000000000000
Al	-0.1412728676843350	-0.0000010707218648	0.0000000000000000

MP2/6-31G** Energy = -241.271433469 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -241.2642241195 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -241.3564268333 a.u.

CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -241.367568514 a.u.

Al³⁺-(H₂)₂

H	1.8261815915264195	-0.3189999217414191	-0.2944947791981833
H	1.8312503284552748	0.2990110071378019	0.2806186987569965
H	-1.8290492626356616	0.2901479310733003	-0.3035813647205156
H	-1.8283497122162544	-0.3093717642431557	0.2909188663247860
Al	-0.0000041167246059	-0.0001191742863843	0.0008052339610704

MP2/6-31G** Energy = -242.537614839 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -242.5085610142 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -242.6365880795 a.u.

CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -242.656128561 a.u.

Al³⁺-(H₂)₃

H	1.1956681496077171	1.4030078040049503	-0.3670725727927738
H	0.9036000611036852	1.6048813931985642	0.3687695856422076
H	-1.8372102319481352	-0.0179001713111755	0.3700184314978787
H	-1.8082997042110101	0.3225424253742042	-0.3721324243097099
H	0.6207789426236363	-1.7350597062623587	-0.3696061046107880
H	0.9464627628642761	-1.5829554214266457	0.3640900341696955
Al	0.0034969750756582	-0.0007371219905997	-0.0009945638425431

MP2/6-31G** Energy = -243.778414096 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -243.7247003829 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -243.8882690477 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -243.915845324 a.u.

Al³⁺-(H₂)₄

H	0.9838843745171663	-0.5967975629583014	1.4913323903626232
H	1.4280266421687018	-0.8531213155691760	0.8774329548707014
H	-1.2273895438649161	-1.0863869378586197	-0.9235987148263601
H	-0.6559699899532669	-1.6095228967303379	-0.7244620342015046
H	-1.0072575298615511	1.4163960450000164	0.7293334411925677
H	-1.3312912425451351	0.7744646350795907	1.0798260929960743
Al	-0.0000257996770357	0.0006252785018211	-0.0003168353067353
H	0.6775513394269423	0.8213551626865676	-1.5545683297297981
H	1.1318822186169220	1.1409745521730845	-0.9789438374261958

MP2/6-31G** Energy = -245.003635896 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -244.9247307078 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -245.1252304049 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -245.160790244 a.u.

Al³⁺-(H₂)₅

H	-0.1066917443272677	1.7825723554651483	0.5738446781779627
H	-0.0630165651985351	1.3765697033972344	1.2480709420099192
H	0.1051337830910286	-1.7807367347275738	0.5872907857232789
H	0.0558667160875336	-1.3702137284362386	1.2583729005514639
H	0.0760062225152309	-0.3943788990831313	-1.9343714567336732
H	-0.0648834967502724	0.3801112931285938	-1.9371799596689752
Al	0.0005906542969380	-0.0014875225912085	-0.0720233255021611
H	1.9016053554926524	-0.2713939891715245	-0.0123006952953399
H	1.8574846615879470	0.4877480464491759	-0.1794960300458441
H	-1.9008701393542218	0.2680342738479684	-0.0251027138101861
H	-1.8554751808231771	-0.4923920493877357	-0.1859771083545943

MP2/6-31G** Energy = -246.199683709 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -246.0963834019 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -246.3359765480 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -246.379558901 a.u.

Al³⁺-(H₂)₆

H	0.6054011780567998	1.5299044226930918	-1.0028259268190935
H	1.1201450884421322	1.5101331084863174	-0.4242466667512331
H	1.4791196456289728	-0.2773515893401864	1.2039963230553972
H	1.0218170134347129	0.1863276691968822	1.6234943164359015
H	-1.4807534924761794	0.2740217226322220	-1.2026400543901885
H	-1.0190673662786598	-0.1821053439363259	-1.6256696633761625
Al	0.0000052071297756	-0.0001950370732160	-0.0000523849617209
H	0.9470624935624610	-1.4304142123915444	-0.8785945401054170
H	1.2965228618231710	-0.8064651842292347	-1.1763702140032031
H	-0.9455277619802892	1.4299884017635511	0.8802531199196924
H	-1.2959827902582322	0.8059082581578404	1.1766510573206261
H	-1.1167048099026207	-1.5136549870238443	0.4209694608838608
H	-0.6075622576760350	-1.5282404404204522	1.0046773679062200

MP2/6-31G** Energy = -247.395695455 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -247.2677205507 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -247.5472442958 a.u.
CCSD(T)/cc-pVTZ//MP2/6-31G** Energy = -247.598601149 a.u.

[Li(CN)]-(H₂)

0 1

Li	1.6395600466803477	0.0012872304732026	0.0001870329350856
C	-0.2873937884544676	0.0003551119795572	0.0000727376742653
N	-1.4768859551782474	-0.0004294920281746	-0.0000763582558941
H	3.7449346791230882	0.3677267848832159	-0.0002430020261374
H	3.7437728638216350	-0.3707605588152925	-0.0002373133063497

MP2/6-31G** Energy = -101.232380311 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -100.9419917567 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -101.3640363375 a.u.

[Li(CO)]⁺-(H₂)

Li	1.8934005601078354	0.0011939914763087	0.0000071007075849
C	-0.3163199408308344	0.0002820744306447	0.0000015555906815
O	-1.4580422223365359	-0.0002897744135600	-0.0000017426344496
H	3.9617938098918057	0.3691812981621093	-0.0000081198498415
H	3.9608032395738229	-0.3719961565271656	-0.0000079592181052

MP2/6-31G** Energy = -121.460239630 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -121.1759699295 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -121.6105038209 a.u.

[Li(CO)₂]⁺-(H₂)

Li	-0.0003260028567207	-0.6517076355279463	-0.0000820224144235
C	-2.1407386852751040	-0.0378310753422392	0.0000641524633721
O	-3.2383074027264964	0.2785276028109352	0.0001611935829575
C	2.1403153304954965	-0.0386057224555821	-0.0000122732960405
O	3.2380007820926640	0.2773479380683253	0.0000022966587728
H	0.3691834056522109	-2.7828617976870658	-0.0009985715345375
H	-0.3702221182683533	-2.7828257629357798	0.0006156105883787

MP2/6-31G** Energy = -234.515859366 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -233.9698045626 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -234.7963636627 a.u.

[Li(CO)₃]⁺-(H₂)

Li	-0.0013316162600176	0.0227930193064421	0.4576378207769373
C	1.8896996929203194	1.1315103888410851	-0.0115578382848622
C	-1.9332363626200839	1.0581564554235536	-0.0120251826065090
C	0.0426982023655401	-2.1739109840270996	0.0000124616485645
O	2.8524728994216972	1.6976492089449924	-0.2542711233331009
O	-2.9169151750735685	1.5868878541252447	-0.2552756907343681
O	0.0650647249804769	-3.2931993308741658	-0.2304601619220394
H	0.3687269650267868	0.0088960288172556	2.6246837060278900
H	-0.3698616673123671	0.0099344079558977	2.6250267422174489

MP2/6-31G** Energy = -347.568474304 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -346.7603642208 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -347.9790926867 a.u.

[Mg(CN)]⁺-(H₂)

Mg 1.0909418494762779 0.0037808963827678 -0.0375668259524271
C -0.8955351878482630 -0.0010821152907380 -0.0057233360318496
N -2.0837415228123257 -0.0044223652902194 0.0131661206921442
H 3.1957008350540255 0.3803248248835963 -0.0707696210665428
H 3.1959541258274986 -0.3700557262086734 -0.0729395481569668

MP2/6-31G** Energy = -293.108973052 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -292.8204205533 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -293.2577939540 a.u.

[Mg(CN)₂]- (H₂)

0 1

Mg -0.0251202558280423 0.0786519500127928 -0.0022744394657267
C -2.0617811215793402 0.2675373220492411 0.0305302485917652
C 2.0178391692464870 0.1805160862045745 -0.0301869207174554
N 3.2034989493718729 0.2349450445199071 -0.0464828188764583
N -3.2440121997450628 0.3723594974019366 0.0494602545756614
H 0.2938763165990187 -2.2909911034418537 -0.0469486404635278
H -0.4459317795645854 -2.2758537041081190 -0.0364837706987836

MP2/6-31G** Energy = -386.024319062 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -385.4659813926 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -386.2854258523 a.u.

[Mg(CO)]²⁺-(H₂)

Mg 1.2669424141878445 -0.0039196760739195 0.0392287722213096
C -0.9653659313611089 0.0014157578945928 0.0036415099458364
O -2.1045494007077812 0.0042473427210622 -0.0145177280762156
H 3.3172935250233513 -0.3850945099219930 0.0708146511596390
H 3.3176415070491796 0.3748286875218731 0.0730851602741244

MP2/6-31G** Energy = -313.116454504 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -312.8364929773 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -313.2864735422 a.u.

[Mg(CO)₂]²⁺-(H₂)

Mg 0.0090337703022072 -0.6458795245774288 -0.0172819622437968
C -2.0538956628479159 0.2737968658276980 -0.0322616373415400
O -3.0923113197820462 0.7433362052903623 -0.0396515606885118
C 2.0618508291296251 0.2949693105803071 0.0292561130283195
O 3.0951007365963097 0.7752491749236440 0.0527890784376148
H 0.3957693368004480 -2.7199340107301127 -0.0500951318168862
H -0.3576775720478170 -2.7233194375195016 -0.0579722138656266

MP2/6-31G** Energy = -426.214258949 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -425.6651020565 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -426.5141046382 a.u.

[Mg(CO)₃]²⁺-(H₂)

Mg -0.0000422853312047 0.0007886576581356 0.4413595192872953
C 1.9008862512294045 1.1438232039829823 -0.0932474571795986
C -1.9440498200466365 1.0689605322764737 -0.0932742313439042
C 0.0433662610471384 -2.2165912456108705 -0.0923330856670761
O 2.8488745159255422 1.7158111167968033 -0.3657329704096690
O -2.9135746362253205 1.6035320081136313 -0.3659606728811911
O 0.0649963827231052 -3.3246744492024449 -0.3601705940241370
H 0.3730960026980643 0.0274116959550900 2.5566487027550484
H -0.3761674084874389 0.0283182801096646 2.5560199190550796

MP2/6-31G** Energy = -539.302333178 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -538.4835412992 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -539.7312026133 a.u.

[Al(CN)]²⁺-(H₂)

Al -1.0959024374996431 0.0031568579946329 0.0396533793933364
C 0.7233881723206256 -0.0011863224571810 0.0110172352905579
N 1.9248948204122067 -0.0042037383303916 -0.0079732951146741
H -2.9370257706713376 0.4011752841745470 0.0673065237127162
H -2.9380690401109724 -0.3901842475671002 0.0702060488215119

MP2/6-31G** Energy = -334.804305843 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -334.4994215007 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -334.9959542444 a.u.

[Al(CN)₂]⁺-(H₂)

Al -0.0310683246508537 -0.1831353113134840 -0.0079051346294810
C -1.8412977802502579 0.2142663905624086 0.0306445187761503
C 1.7954214391279228 0.1324624316414525 -0.0358261016493022
N 2.9689519725991875 0.3261617598147191 -0.0536463967815868
N -3.0047941664483249 0.4606432743051564 0.0548994822129643
H 0.3027229307976235 -2.1396332881595472 -0.0437561191214952
H -0.4518941614486507 -2.1229644388963340 -0.0302028936598494

MP2/6-31G** Energy = -428.019440736 a.u.

HF/cc-pVTZ//MP2/6-31G** Energy = -427.4379408890 a.u.

RIMP2/cc-pVTZ//MP2/6-31G** Energy = -428.3203157779 a.u.

[Al(CN)₃]⁻-(H₂)

0 1

Al 0.0073932656438336 -0.0040953804900455 -0.0487849852977933
C 0.6483569658482029 -1.7978423342464045 0.0954827722146895
C -1.8695536326761404 0.3378767689797991 0.0719193677595014
C 1.2446906239482332 1.4453392354811829 0.0884522071345513
N -3.0348334941651331 0.5488141271761443 0.1304537824605639
N 1.0476920595061676 -2.9106069659745222 0.1842998159541449
N 2.0149552877548325 2.3431336760547246 0.1678934896730776
H 0.3424264382607011 0.0178604051104909 -2.1735684942617359
H -0.4003642487001567 0.0180132645065068 -2.1562874717234077

MP2/6-31G** Energy = -520.974726260 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -520.1232603055 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -521.3853731004 a.u.

[Al(CO)]³⁺-(H₂)

Al	-1.2401443969457628	0.0036871967054277	0.0405312485507395
C	0.7915082623299714	-0.0015628180996581	0.0084636817591189
O	1.9367174238232832	-0.0045254799113075	-0.0096069312919717
H	-3.0674530125447572	0.4201143742466745	0.0680183009599512
H	-3.0683968904163410	-0.4089780265588545	0.0712657070231065

MP2/6-31G** Energy = -354.523468766 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -354.2274445346 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -354.7413358163 a.u.

[Al(CO)₂]³⁺-(H₂)

Al	-0.0003376855582019	-0.7178139567605578	-0.0002518249169987
C	-1.8603896844908749	0.1458115188206730	-0.0000265057207841
O	-2.8941608181131562	0.6332903059629154	0.0000856350947092
C	1.8600000933116125	0.1451982316779795	-0.0000843386666334
O	2.8939216043192504	0.6323579670404059	0.0000253380892583
H	0.3959979585083826	-2.5608692967717621	-0.0017691724127591
H	-0.3972279895020637	-2.5607276368827585	0.0006731537407815

MP2/6-31G** Energy = -467.720747595 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -467.1423648103 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -468.0683324600 a.u.

[Al(CO)₃]³⁺-(H₂)

Al	-0.0014834602631343	-0.0098225625830670	0.4383403350819560
C	1.7173167279264798	1.0311395773290279	-0.0698184509197992
C	-1.7550710147295212	0.9689135730696536	-0.0747715959984495
C	0.0348691568381379	-2.0120464579385251	-0.0922657456596075
O	2.6615203551168909	1.6047967806461465	-0.3575227961875656
O	-2.7183990904808719	1.5083243923733993	-0.3653234090405768
O	0.0548425642620202	-3.1141215082371323	-0.3893011421492035
H	0.3845847834753223	-0.0298551789521671	2.3049738021182558
H	-0.3914171489184116	-0.0285797057437194	2.3045026500130583

MP2/6-31G** Energy = -580.882126462 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -580.0254936591 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -581.3602418706 a.u.

[Li(CO)₃]⁺-(H₂)₂

Li	0.0022492152161417	0.0022906466466335	0.0000528107584495
C	0.5267259229917585	2.1894264799280845	0.0025448647220907
C	1.5979251847806581	-1.5842488135108113	-0.0043687008461352
C	-2.1547071526295536	-0.6404047582220591	0.0021419962217171
O	0.7960355933424249	3.3003108439162530	0.0015059264081476
O	2.4128997825283194	-2.3857450290956517	-0.0014169377648404
O	-3.2511243055206451	-0.9635834845679317	0.0005365968979338
H	-0.1200030541509562	0.3543604343427971	-2.3494527431197239

H 0.0811024461827848 -0.3547771496828461 -2.3494456513434865
H 0.0978031824308995 0.3363744319118087 2.3541726063158932
H -0.0934353300086726 -0.3754291229407788 2.3451002273437065

MP2/6-31G** Energy = -348.727981395 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -347.8939085206 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -349.1462115381 a.u.

[Mg(CO)₃]²⁺-(H₂)₂

Mg 0.0330213913986175 -0.0052003056340693 0.1177036547149115
C 1.9570618571178158 1.2392833828727232 0.1665356762593455
C -2.0009713361909696 1.0484627824775929 0.0427420682446355
C 0.1413594290874446 -2.2933606960979684 0.1450192670634129
O 2.9110031734529138 1.8636390280419837 0.1913101237314846
O -3.0108133749747412 1.5770150169158728 0.0063102080410491
O 0.1940324323328991 -3.4323342663968526 0.1592664395734465
H 0.3394612120028337 0.0017330012058889 2.3190941162643313
H -0.4048741880382309 0.0271667835401232 2.2964707634480623
H 0.4793536348959271 -0.0456719775256789 -2.0592296402003134
H -0.2646442026809598 -0.0125160961495509 -2.0840181344289430

MP2/6-31G** Energy = -540.469291491 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -539.6255199748 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -540.9074764996 a.u.

[Al(CO)₃]³⁺-(H₂)₂

Al 0.0187417170628649 -0.0010075709882276 0.0625562095596895
C 1.6885378986342447 -1.2562748158034054 0.1130599591254358
C 0.3251073945461946 2.0641042897533195 0.0664271127991767
C -1.8983894291977370 -0.8214081819920589 0.0107901266783835
O 2.6020970226082354 -1.9398669954890511 0.1427942153713180
O 0.4977811111828088 3.1922281679851645 0.0652244072180691
O -2.9462087249595252 -1.2726320175733061 -0.0154983004217284
H 0.0883410949283806 -0.3535507727443236 2.0167983258210458
H -0.2019134402213161 0.3488277968591695 2.0069354283464342
H 0.3635542807937954 -0.2150733039118159 -1.8816794487483546
H -0.2515472375169092 0.2312896611810865 -1.8932913465212506

MP2/6-31G** Energy = -582.058392034 a.u.
HF/cc-pVTZ//MP2/6-31G** Energy = -581.1804935911 a.u.
RIMP2/cc-pVTZ//MP2/6-31G** Energy = -582.5513236806 a.u.