

Electronic Supplementary Information

Copper (I)-Catalyzed Asymmetric Aza Diels-Alder Reaction of Azoalkenes Toward Fulvenes: A Molecular Electron Density Theory Study

Saeedreza Emamian,^{*a} Mousa Soleymani^b and Samira Sadat Moosavi^a

^a*Chemistry Department, Shahrood Branch, Islamic Azad University, Shahrood, Iran.*

^b*Chemistry Department, Faculty of Science, Ayatollah Boroujerdi University, Borujerd, Iran.*

*Corresponding author. Tel.: +98 9121735085; Fax: +98 2332390537.

E-mail address: s_emamian@iau-shahrood.ac.ir & saeedreza_em@yahoo.com

ORCID ID: <https://orcid.org/0000-0001-8223-1264>

Contents

- S2** B3LYP/6-31G(d) Cartesian coordinates of optimized structures in the presence of DCM involved in the uncatalyzed as well as catalyzed studied ADA reaction.
- S18** Values of different terms employed in equation (1) for the located stationary points (Table S1).

AD-2

C	-1.68775700	0.96133300	0.67077400
C	-1.71840300	1.79690000	1.72485200
H	-0.83729100	2.36591200	2.00309100
H	-2.62777100	1.96506100	2.29201600
N	0.56835800	0.97377900	0.43081600
N	-0.52842500	0.89591300	-0.16288500
C	-2.82919900	0.15353100	0.17589500
C	-3.83602000	-0.27348500	1.05910400
C	-2.92266200	-0.20914500	-1.17951900
C	-4.91612500	-1.02301500	0.59666100
H	-3.76268300	-0.03344500	2.11590100
C	-4.00509700	-0.96043800	-1.63814400
H	-2.15146300	0.10889500	-1.87241600
C	-5.00661800	-1.36864600	-0.75491900
H	-5.68314600	-1.34667100	1.29523900
H	-4.06482700	-1.22529400	-2.69052500
H	-5.84698400	-1.95667300	-1.11403000
C	1.70214800	1.07335200	-0.46879100
O	1.71007500	1.89893300	-1.36455100
C	2.83306500	0.17963400	-0.13198300
C	2.79042400	-0.69058200	0.97058400
C	3.96371600	0.19213100	-0.96697200
C	3.86667400	-1.53808100	1.22941200
H	1.92319300	-0.69519300	1.62256500
C	5.03530900	-0.65471500	-0.70315900
H	3.98363500	0.86760600	-1.81631200
C	4.98753500	-1.52124600	0.39499400
H	3.83202500	-2.20943500	2.08268200
H	5.90763300	-0.64347700	-1.35053600
H	5.82561700	-2.18177900	0.60048700

FU-3

C	0.97253600	1.17338400	-0.00363900
C	2.25924700	0.73218100	-0.00378100
C	2.25925200	-0.73217500	0.00378700
C	0.97254300	-1.17339000	0.00363000
H	0.64646000	2.20586300	-0.01425100
H	3.15120200	1.35034000	-0.00980900
H	3.15120600	-1.35033500	0.00982800
H	0.64650400	-2.20588100	0.01420500
C	0.08319100	-0.00000900	0.00000300
C	-1.28024500	0.00000500	0.00001700
C	-2.09767000	1.26157800	0.00746200
H	-2.69195100	1.33074800	-0.91468600
H	-2.82027300	1.23896600	0.83463000
H	-1.49893300	2.16940800	0.09841000
C	-2.09769200	-1.26156800	-0.00745600
H	-1.49893600	-2.16937400	-0.09855400
H	-2.69193600	-1.33087900	0.91470200
H	-2.82030500	-1.23889300	-0.83461400

TS-1x

C	-2.07871100	-0.22510200	0.60312600
C	-1.64668300	0.94402600	1.25162100
H	-0.66741600	0.92986600	1.71276100
H	-2.37446600	1.60327200	1.71036200
N	0.07035300	-0.85070700	0.30183900
N	-1.18168100	-1.10018400	0.07618400
C	-3.50185900	-0.50109000	0.28816600

C	-4.55020400	0.13630400	0.97950000
C	-3.84410700	-1.42231000	-0.72276300
C	-5.88371600	-0.12584800	0.66466600
H	-4.32970800	0.82883800	1.78644300
C	-5.17682700	-1.68811300	-1.02982200
H	-3.04942500	-1.92079400	-1.26688600
C	-6.20621000	-1.03901900	-0.34165200
H	-6.67260100	0.37895900	1.21660200
H	-5.41256100	-2.40002300	-1.81702500
H	-7.24535800	-1.24448300	-0.58477200
C	0.92556700	-1.69963700	-0.44455700
O	0.61141200	-2.24428900	-1.49998200
C	2.29837200	-1.84442800	0.13448700
C	2.68809600	-1.21645500	1.32916500
C	3.22207300	-2.65722500	-0.54398500
C	3.97809600	-1.39764400	1.82981500
H	1.98007300	-0.58882200	1.85773200
C	4.50856100	-2.83708300	-0.04268500
H	2.91078600	-3.14075700	-1.46442100
C	4.89027900	-2.20570300	1.14625200
H	4.27080200	-0.90777800	2.75471700
H	5.21497800	-3.46828700	-0.57540200
H	5.89466100	-2.34466000	1.53783100
C	-1.08727800	2.36782800	-0.20534300
C	0.04100200	1.83177800	-0.84816200
C	0.72998300	3.58368300	0.53601400
H	-2.08472300	2.32014200	-0.62827300
H	0.01593800	1.08041400	-1.62378800
H	1.35994400	4.28607800	1.06720000
C	-0.61742000	3.49810600	0.62320900
C	1.21539600	2.56088800	-0.41074300
C	2.49895000	2.39088600	-0.86454800
H	-1.26676100	4.11621900	1.23346000
C	2.86964400	1.36554400	-1.89393900
H	3.16432300	1.87277100	-2.82425600
H	3.74952700	0.79885200	-1.56515300
H	2.06880200	0.66286700	-2.12678500
C	3.64005400	3.24549100	-0.39928900
H	3.34625800	4.03223600	0.29687100
H	4.39889000	2.61685000	0.08732800
H	4.13769400	3.70952500	-1.26204900

TS-1n

C	-1.62984000	-1.02509800	0.56493000
C	-1.42405700	-0.82892800	1.93837500
H	-0.46738000	-1.12028100	2.35388700
H	-2.26817600	-0.87012300	2.61754200
N	0.59269400	-0.86967500	0.22099800
N	-0.58937300	-0.96170000	-0.30668700
C	-2.97440200	-1.14488300	-0.04994400
C	-4.08566900	-1.58738400	0.69191800
C	-3.16877600	-0.83365800	-1.41037700
C	-5.34511500	-1.69803500	0.10149400
H	-3.96644200	-1.87209100	1.73344300
C	-4.42549800	-0.95323800	-1.99991700
H	-2.32160300	-0.49098200	-1.99459300
C	-5.52318100	-1.38101800	-1.24698100
H	-6.18649600	-2.04477800	0.69620600
H	-4.55019700	-0.70225300	-3.05040700
H	-6.50370600	-1.47035400	-1.70718500
C	1.59156700	-0.58804000	-0.73869600
O	1.38702800	0.02616600	-1.78361700

C	2.96158800	-1.05347000	-0.35244100
C	3.21998800	-1.72474600	0.85429300
C	4.01553900	-0.84389900	-1.25723700
C	4.50919500	-2.16922700	1.14970800
H	2.40970000	-1.89473200	1.55404200
C	5.30108600	-1.29022600	-0.96186700
H	3.80562900	-0.33111200	-2.19051600
C	5.55117200	-1.95430900	0.24381700
H	4.69997400	-2.68671600	2.08621900
H	6.10865600	-1.12426900	-1.67001500
H	6.55451200	-2.30242100	0.47527200
C	0.21325200	1.52898100	1.64461800
C	-1.00443800	1.23278600	2.28448700
C	-2.06264300	1.96291100	1.56105400
C	-1.51777000	2.58812600	0.49241500
H	1.19139400	1.26768900	2.02206500
H	-1.05912000	0.99662600	3.34213600
H	-3.11345200	1.93470100	1.82662800
H	-2.05523600	3.15934700	-0.25404300
C	-0.05597100	2.38576200	0.50735000
C	0.87123400	2.96555100	-0.32144400
C	2.35041400	2.79283700	-0.13826200
H	2.82986600	2.57294800	-1.09868300
H	2.78529000	3.73867400	0.21715800
H	2.61695700	2.00910800	0.57175100
C	0.48715900	3.87211400	-1.45291400
H	-0.58101300	4.08953000	-1.49877400
H	1.03642900	4.82098300	-1.38377300
H	0.78593600	3.41334300	-2.40587100

CA-1x

C	2.23735200	0.17895700	-0.26717900
C	1.73157800	1.38571300	-1.02075800
H	1.32413300	1.01901600	-1.97328600
H	2.52505900	2.09698600	-1.25357800
N	0.04925700	-0.31927000	0.06155200
N	1.39966500	-0.66975700	0.23273500
C	3.68198600	-0.12325100	-0.11699700
C	4.64925500	0.49269700	-0.92968300
C	4.11148100	-1.06169800	0.84176800
C	6.00221600	0.17646200	-0.79230500
H	4.35179300	1.20899900	-1.68888900
C	5.46097000	-1.37367800	0.97782100
H	3.37246800	-1.53581600	1.47904900
C	6.41422500	-0.75511900	0.16152400
H	6.73311600	0.65964500	-1.43536400
H	5.77258200	-2.09684600	1.72701600
H	7.46813000	-0.99669700	0.27124600
C	-0.80731100	-1.42407300	0.28940100
O	-0.43231000	-2.44165400	0.85718900
C	-2.16166300	-1.37769900	-0.34929600
C	-2.38762800	-0.73932100	-1.57736100
C	-3.19473800	-2.12719800	0.23539200
C	-3.63559100	-0.82786800	-2.19590900
H	-1.58436800	-0.18545500	-2.04999600
C	-4.44614700	-2.19803800	-0.37343900
H	-3.00420700	-2.64937700	1.16788500
C	-4.66913200	-1.54794600	-1.59173500
H	-3.79899700	-0.33712000	-3.15175900
H	-5.24444000	-2.76724000	0.09533000
H	-5.64196700	-1.61148300	-2.07226000
C	0.60166300	2.07960100	-0.23046400

C	-0.22486700	1.06798000	0.60880200
C	-1.68675800	2.49670500	-0.63150300
H	1.06113700	2.80159500	0.45941600
H	0.13210000	1.03656400	1.64330400
H	-2.59647600	2.91592200	-1.04772600
C	-0.44689000	2.77252200	-1.06920500
C	-1.65546800	1.59283100	0.52897000
C	-2.62646000	1.40034300	1.44980800
H	-0.19745900	3.43610400	-1.89236000
C	-2.45659800	0.53028000	2.66840200
H	-2.63864600	1.11436900	3.58198700
H	-3.19984600	-0.27882200	2.66909300
H	-1.46671100	0.07530900	2.75276200
C	-3.98821800	2.04043900	1.34720300
H	-4.10804600	2.67424200	0.46581100
H	-4.77117500	1.26968600	1.31943700
H	-4.19171000	2.65501100	2.23581700

CA-1n

C	-1.67910400	-0.73931000	0.26944300
C	-1.20092500	-0.97897900	1.68425300
H	-0.65138600	-1.93037100	1.69295000
H	-2.02824000	-1.06766000	2.39037400
N	0.49159100	-0.35574600	-0.18070300
N	-0.82612700	-0.47311700	-0.66693300
C	-3.10810600	-0.82043500	-0.11529100
C	-4.03518700	-1.53642900	0.66149300
C	-3.55786300	-0.19287600	-1.29275800
C	-5.37147100	-1.62716000	0.26867600
H	-3.71594900	-2.04539600	1.56551600
C	-4.89230300	-0.28084400	-1.67907000
H	-2.84982400	0.37065100	-1.89111500
C	-5.80569000	-0.99828900	-0.89941500
H	-6.07249300	-2.19118700	0.87809600
H	-5.22336200	0.21664200	-2.58684500
H	-6.84820800	-1.06272200	-1.19952700
C	1.47160200	-0.90387900	-0.98366300
O	1.21906400	-1.38365200	-2.08779600
C	2.87333700	-0.99959700	-0.43773500
C	3.15395300	-1.44550800	0.86251000
C	3.93587900	-0.77622400	-1.32691200
C	4.47505500	-1.63803700	1.27230300
H	2.34097900	-1.66766900	1.54750300
C	5.25462100	-0.95161200	-0.91103700
H	3.71619300	-0.46737400	-2.34426500
C	5.52746800	-1.38299900	0.39066300
H	4.67993500	-1.99361100	2.27855400
H	6.06918900	-0.76113300	-1.60464700
H	6.55531100	-1.52861900	0.71228900
C	0.66249800	0.59900500	0.93587100
C	-0.24460800	0.15951200	2.13117600
C	-0.99525300	1.41514500	2.49174200
C	-0.76225800	2.41540800	1.62738100
H	1.71497600	0.58355900	1.21481000
H	0.35551500	-0.21194900	2.97083600
H	-1.67426400	1.45853700	3.33847100
H	-1.22148200	3.39622900	1.68874200
C	0.21943700	2.04757400	0.60600600
C	0.68588100	2.83696100	-0.38738300
C	1.76599600	2.41021800	-1.35082200
H	1.34021000	2.00366200	-2.27970700
H	2.37804900	3.27441700	-1.63901300

H	2.43727100	1.65656200	-0.93347000
C	0.15828400	4.22782900	-0.64443200
H	-0.70144600	4.49572400	-0.02620000
H	0.94422100	4.97881100	-0.47861100
H	-0.14340900	4.32731700	-1.69692400

TS-2x

C	-1.15817700	-1.00164300	0.48077900
C	-1.25100000	0.34875600	0.82856600
H	-0.36622000	0.85434000	1.19544700
H	-2.20412400	0.75756400	1.14138800
N	1.07174800	-0.80156600	0.16559400
N	0.02468900	-1.55464300	0.08530400
C	-2.34112900	-1.89078100	0.35889900
C	-3.52281200	-1.64727100	1.08371500
C	-2.30524900	-3.01580600	-0.48842200
C	-4.62793600	-2.48970800	0.95946500
H	-3.57421100	-0.80915000	1.77287500
C	-3.40839300	-3.85936300	-0.60653900
H	-1.40145900	-3.21767900	-1.05339000
C	-4.57850400	-3.59959400	0.11275900
H	-5.52646400	-2.28252500	1.53538900
H	-3.35650100	-4.71878900	-1.27046900
H	-5.43887600	-4.25695900	0.01864300
C	2.20279900	-1.38629700	-0.46281500
O	2.13634800	-2.21543800	-1.36599600
C	3.51306800	-0.85603000	0.02501000
C	3.60974300	0.09659800	1.05311800
C	4.68988700	-1.35995600	-0.55378600
C	4.86045700	0.53629800	1.48827500
H	2.70527000	0.48925700	1.50318700
C	5.93688500	-0.92039100	-0.11764500
H	4.60516800	-2.09764600	-1.34538300
C	6.02510900	0.02936900	0.90598600
H	4.92591500	1.27441700	2.28328800
H	6.84088200	-1.31720000	-0.57204500
H	6.99834100	0.37305700	1.24674300
C	-1.17453100	1.58392200	-1.00580100
C	0.13598700	1.37318900	-1.45188500
C	0.95093900	2.49183700	-1.06567600
C	0.16087300	3.43133800	-0.45502700
H	-2.03666400	1.08046600	-1.42319400
H	0.46951700	0.53243000	-2.04531200
H	2.02044000	2.56420300	-1.22722700
H	0.50430800	4.36690200	-0.03169900
C	-1.21918500	2.95738100	-0.43988700
C	-2.32652500	3.64679500	-0.04184000
C	-3.70476900	3.05090400	-0.06098100
H	-4.13735600	3.07986900	0.94884500
H	-4.36810600	3.65662700	-0.69376100
H	-3.73276400	2.02077500	-0.41935900
C	-2.27262800	5.06917700	0.43826900
H	-2.69925400	5.14171300	1.44798400
H	-1.26548600	5.48869500	0.45702600
H	-2.89765100	5.70425200	-0.20451400

TS-2n

C	-0.75093300	0.68518000	-0.79730800
C	-0.72345600	-0.41350200	-1.65496300
H	0.23129100	-0.73348100	-2.05080300

H	-1.60022700	-0.68380900	-2.23107700
N	1.44384300	0.40275300	-0.32911100
N	0.35657400	1.05080500	-0.07976600
C	-1.97664800	1.47590400	-0.51551100
C	-3.07903000	1.45939400	-1.38970900
C	-2.05757200	2.28789000	0.63295400
C	-4.22803100	2.20245100	-1.11315200
H	-3.03573500	0.88051500	-2.30768500
C	-3.20166100	3.03548000	0.90295500
H	-1.21432100	2.31509100	1.31444200
C	-4.29743000	2.99387600	0.03516100
H	-5.06450400	2.17277400	-1.80706700
H	-3.24047400	3.64880100	1.79990000
H	-5.19045300	3.57529300	0.24892100
C	2.46999700	0.68604800	0.60793200
O	2.26681900	1.08787700	1.75061100
C	3.84748900	0.37086400	0.11754700
C	4.10668300	-0.03073700	-1.20346100
C	4.92022600	0.50837400	1.01399800
C	5.41457700	-0.28617600	-1.61656200
H	3.28308600	-0.13864200	-1.90021300
C	6.22445900	0.24869100	0.60126900
H	4.71029400	0.82148100	2.03177100
C	6.47458500	-0.14952400	-0.71635100
H	5.60653400	-0.59301800	-2.64133800
H	7.04684500	0.35592000	1.30365900
H	7.49249300	-0.35209600	-1.03933100
C	0.33929100	-2.16458900	0.36951900
C	-0.80823200	-2.29159500	-0.41811700
C	-1.40197900	-1.54259500	1.71303800
H	1.34548200	-2.41967800	0.06223700
H	-0.85725100	-2.88630800	-1.32164400
H	-1.96788200	-1.15824400	2.55212100
C	-0.03488700	-1.66251700	1.65840300
C	-1.97338200	-2.01031100	0.45690000
C	-3.29175800	-2.18755100	0.15862500
C	-3.76005400	-2.68737900	-1.17840400
H	-4.32228200	-3.62331800	-1.05363100
H	-4.45978100	-1.96797900	-1.62497200
H	-2.94909700	-2.86737400	-1.88608800
C	-4.39499700	-1.91113100	1.13978400
H	-4.03955700	-1.56632600	2.11206900
H	-5.07478900	-1.15107000	0.73058400
H	-4.99908900	-2.81573900	1.29285200
H	0.65839900	-1.38998300	2.44525800

CA-2x

C	-1.76555400	-0.44584100	0.04021000
C	-1.58115700	1.04760700	-0.03760000
H	-1.77898300	1.47130400	0.95584300
H	-2.32892000	1.48081400	-0.70878100
N	0.51138900	-0.88624900	0.09016900
N	-0.80043900	-1.29793000	0.09779900
C	-3.13971600	-1.01817800	0.06912800
C	-4.26280700	-0.20290400	0.29144500
C	-3.34402000	-2.39892100	-0.12140800
C	-5.54790600	-0.74947300	0.32299000
H	-4.14286700	0.86363400	0.45285300
C	-4.62567100	-2.94003600	-0.09457700
H	-2.48346000	-3.03591300	-0.29608700
C	-5.73617900	-2.11796000	0.12829600
H	-6.40142100	-0.10073000	0.50180400

H	-4.76099000	-4.00712900	-0.25134900
H	-6.73652300	-2.54216700	0.14803400
C	1.41265500	-1.91207200	-0.20480300
O	1.04881100	-3.03667400	-0.52566500
C	2.88399300	-1.60189500	-0.11498400
C	3.50248100	-1.28968000	1.10335600
C	3.67169700	-1.77601000	-1.26282700
C	4.88936800	-1.13634000	1.16713200
H	2.90546300	-1.19632300	2.00541800
C	5.05354400	-1.60014700	-1.20043100
H	3.19624800	-2.04539900	-2.20178800
C	5.66559300	-1.28126200	0.01542000
H	5.36220000	-0.90753700	2.11849100
H	5.65352000	-1.72265400	-2.09821400
H	6.74370600	-1.15421500	0.06558300
C	-0.17244900	1.46882600	-0.51088200
C	0.90505300	0.53661300	0.09549300
C	1.19050400	1.20534300	1.42997400
C	0.85103100	2.50477200	1.37043600
H	-0.12915900	1.45172400	-1.60201700
H	1.80769600	0.59464900	-0.52101900
H	1.69595600	0.71489800	2.25340600
H	1.04940600	3.22850300	2.15401400
C	0.17847200	2.82669800	0.10254300
C	-0.11215400	4.04646400	-0.40004600
C	-0.83414800	4.24609100	-1.70927800
H	-1.77444300	4.79414300	-1.55135800
H	-0.23386100	4.86185800	-2.39448400
H	-1.07378000	3.31057300	-2.22094600
C	0.25535600	5.33183700	0.29946300
H	-0.64269700	5.93327200	0.50066900
H	0.77738500	5.17870400	1.24705700
H	0.90046300	5.94944600	-0.34189500

CA-2n

C	-1.27194400	0.77581700	-0.46890100
C	-1.07620900	-0.45678600	-1.31836400
H	-0.56342800	-0.14001700	-2.23797800
H	-2.02696300	-0.90463100	-1.60733000
N	0.95218800	0.68779700	-0.07579700
N	-0.26475700	1.35780600	0.09573300
C	-2.60194500	1.40352600	-0.28155100
C	-3.63019400	1.23266000	-1.22450700
C	-2.84852000	2.21023300	0.84509200
C	-4.86578400	1.85779900	-1.04930500
H	-3.46379500	0.63124400	-2.11296300
C	-4.08424100	2.82757300	1.02048500
H	-2.06170900	2.33637700	1.58151500
C	-5.09906500	2.65380700	0.07365300
H	-5.64573800	1.72248400	-1.79395600
H	-4.25976100	3.44003600	1.90105200
H	-6.06418600	3.13382000	0.21242000
C	2.07615700	1.47992200	0.14357300
O	1.99794600	2.67148500	0.42285300
C	3.42511800	0.84308700	-0.05909900
C	3.74186900	0.10781100	-1.21112600
C	4.42740100	1.10614100	0.88546100
C	5.03926500	-0.36949100	-1.40533800
H	2.97920100	-0.07255300	-1.96361200
C	5.71759100	0.61096600	0.69912300
H	4.18738300	1.69971100	1.76272200
C	6.02648700	-0.12738300	-0.44701700

H	5.27829200	-0.92768000	-2.30658900
H	6.48384200	0.80695400	1.44431900
H	7.03446100	-0.50519200	-0.59615400
C	0.92898600	-0.77687600	0.20670200
C	-0.18065100	-1.50603100	-0.60775000
C	-0.43640900	-1.94326300	1.74578600
H	1.91900100	-1.15698200	-0.04338600
H	0.26801900	-2.13960900	-1.37829600
H	-0.82949600	-2.31888800	2.68453400
C	0.58079900	-1.07310200	1.64803700
C	-0.92943300	-2.35751200	0.42941500
C	-1.83349000	-3.32749400	0.16395600
C	-2.23178300	-3.72203100	-1.23728800
H	-2.13603700	-4.80933400	-1.36822100
H	-3.28857600	-3.48374600	-1.42800300
H	-1.63379200	-3.24014000	-2.01486000
C	-2.52786400	-4.12786000	1.23878400
H	-2.26559800	-3.82108500	2.25385900
H	-3.61940000	-4.04588000	1.13557800
H	-2.29055100	-5.19695000	1.13937100
H	1.12640000	-0.62810900	2.47467600

AD-2-CuL

C	-0.09503200	-2.11957900	1.89942200
N	-0.83805000	-1.23347100	1.05912400
C	-2.66662300	-0.81481800	-0.12785600
O	-1.98711300	-0.04876400	-0.86215800
C	0.98683900	-1.48357800	2.69370600
C	0.80684100	-0.20859000	3.25760300
C	2.19028400	-2.16604300	2.94284200
C	1.80429600	0.36642500	4.04705700
H	-0.12769600	0.32105600	3.10346800
C	3.18567900	-1.58966400	3.73149600
H	2.34968600	-3.14927800	2.50900500
C	2.99745200	-0.32043000	4.28485400
H	1.64285200	1.34713000	4.48652800
H	4.11081400	-2.13107000	3.90987500
H	3.77328600	0.12866100	4.89879400
Cu	-0.06301300	0.01444800	-0.19740900
C	2.80377000	1.58759600	-1.04457600
C	2.68655200	0.07525900	-1.02001500
O	3.85710300	-0.55077000	-1.17836300
C	2.06606800	-2.09264900	-1.03879900
C	3.60504400	-1.97697300	-0.99897600
C	1.45855400	2.28833700	-1.08308300
O	1.48918100	3.51199700	-1.61932100
C	-0.65277400	3.00710800	-0.73814900
C	0.11418400	4.00269100	-1.63691900
N	1.64528700	-0.66945900	-0.86964000
N	0.33153900	1.88911500	-0.60402300
C	-1.12641900	3.58927300	0.63020500
C	1.47838500	-2.76077700	-2.32120600
C	-4.13426200	-0.88726300	-0.21013900
C	-4.87372900	-1.74483300	0.62554100
C	-4.80856100	-0.08249800	-1.14616600
C	-6.26193400	-1.78979100	0.52451000
H	-4.35643500	-2.37084200	1.34409900
C	-6.19614000	-0.12957600	-1.23945600
H	-4.23303500	0.57064900	-1.79373800
C	-6.92557000	-0.98353000	-0.40511000
H	-6.82769500	-2.45414900	1.17148700
H	-6.71080400	0.49436300	-1.96467400

H	-8.00872900	-1.02229000	-0.48189200
N	-2.04627100	-1.63908900	0.79242700
C	-0.36384200	-3.43988900	1.93044200
H	0.18273500	-4.10591400	2.58949100
H	-1.14231200	-3.86923900	1.31002700
C	3.53398200	2.04518500	0.25322200
H	3.61830700	3.13563700	0.26075700
H	2.99363300	1.72427000	1.14842700
H	4.53992800	1.61780800	0.27581500
C	3.64517300	1.99446100	-2.28188900
H	4.62116900	1.50825800	-2.23876900
H	3.14914300	1.70534600	-3.21380900
H	3.79324400	3.07566700	-2.28713400
H	4.13037200	-2.49762700	-1.79798000
H	4.03041200	-2.26044800	-0.03341800
H	-0.22008200	3.98511400	-2.67716800
H	0.13579500	5.03038900	-1.27708900
H	1.70545900	-2.65739100	-0.17552000
C	-0.05641900	-2.81728600	-2.21514500
H	-0.49786400	-1.81817400	-2.16399500
H	-0.47648000	-3.32389200	-3.09195900
H	-0.37376100	-3.37572500	-1.32616600
C	2.01222600	-4.20643400	-2.39164300
H	1.77913900	-4.76430700	-1.47587900
H	1.54510700	-4.73487600	-3.23067800
H	3.09632200	-4.24713800	-2.54640300
C	1.87570400	-1.99318100	-3.59426200
H	1.48093300	-0.97059300	-3.58697900
H	2.96315600	-1.93966100	-3.72553200
H	1.46728200	-2.49692100	-4.47788600
C	0.05458200	4.13036300	1.45667200
H	-0.31248600	4.55319600	2.39895100
H	0.76777200	3.33705500	1.70847000
H	0.60073500	4.92612800	0.93635700
C	-1.85537300	2.50072200	1.43707900
H	-1.20160900	1.64824700	1.64279700
H	-2.19326800	2.90777700	2.39757300
H	-2.73691800	2.13272700	0.90080200
C	-2.12946000	4.72487800	0.33952500
H	-2.53336300	5.11501000	1.28094200
H	-1.67203900	5.56666200	-0.19251200
H	-2.97357400	4.36349800	-0.26084900
H	-1.52951100	2.61698700	-1.25996700

TS-2x-CuL

C	1.51177000	-1.11007100	-0.20821800
N	0.85221800	0.06746200	-0.00400400
C	0.85799600	2.15544700	0.80699500
O	-0.40722900	2.15316800	0.83343600
C	0.82389700	-2.15063100	-1.01761800
C	0.12573300	-1.81159300	-2.19114000
C	0.91386600	-3.51057600	-0.66651800
C	-0.47259000	-2.79724600	-2.97800300
H	0.08355300	-0.77433100	-2.50631400
C	0.31199400	-4.49485000	-1.45184900
H	1.44740300	-3.79870200	0.23547600
C	-0.38623100	-4.14257000	-2.60974000
H	-0.99396200	-2.51401400	-3.88871100
H	0.38808900	-5.53820300	-1.15717400
H	-0.85186900	-4.90922500	-3.22293200
Cu	-1.07411700	0.31570800	0.20384700
C	-4.14998900	-1.10787200	-0.05553000

C	-3.06635100	-1.66742800	0.84925900
O	-3.37561200	-2.87065000	1.35729200
C	-1.30599000	-2.07856500	2.18807000
C	-2.20550400	-3.33043200	2.09452200
C	-3.87686300	0.31310900	-0.51588100
O	-4.97874800	1.00138800	-0.84990100
C	-3.00271200	2.24197800	-1.28384200
C	-4.54504100	2.34341000	-1.21742500
N	-1.93062200	-1.16510800	1.18808800
N	-2.74411600	0.89799700	-0.68617300
C	-2.39194000	2.42186200	-2.70775700
C	-1.18900100	-1.44263400	3.60850700
C	1.60408100	3.40043700	1.12486300
C	2.98417200	3.39273900	1.38838400
C	0.90467500	4.61746800	1.18253100
C	3.64824700	4.57952500	1.69545700
H	3.52709100	2.45520800	1.36482400
C	1.57364400	5.80364800	1.47733500
H	-0.16332700	4.61926000	0.99167900
C	2.94763300	5.78844200	1.73532300
H	4.71411000	4.56101500	1.90711300
H	1.02337200	6.74014900	1.51066600
H	3.46848000	6.71261500	1.97144900
N	1.59812500	1.05435500	0.50571000
C	2.83776300	-1.30601100	0.20381200
H	3.23768200	-2.31090700	0.15570700
H	3.26616600	-0.65024000	0.95083000
C	-4.24367000	-2.00552900	-1.32414100
H	-5.00609200	-1.60889200	-2.00096300
H	-3.28702900	-2.04483000	-1.85291600
H	-4.52724000	-3.02142800	-1.03662900
C	-5.49693000	-1.15911200	0.71226400
H	-5.70314700	-2.18372900	1.02692500
H	-5.47534800	-0.51817700	1.59949600
H	-6.30674400	-0.82335200	0.06201300
H	-2.55818100	-3.71967800	3.04899300
H	-1.75269700	-4.13824200	1.51420500
H	-4.89577500	3.02323600	-0.43690000
H	-5.03249900	2.59202700	-2.15938700
H	-0.29448100	-2.31235600	1.84503600
C	-0.25330000	-0.22217100	3.54667400
H	-0.62677300	0.53646900	2.85390900
H	-0.16536700	0.23838200	4.53793000
H	0.75509100	-0.50907200	3.22444000
C	-0.56379300	-2.48908400	4.55319200
H	0.39734600	-2.85151600	4.16680900
H	-0.37934700	-2.04134500	5.53669900
H	-1.21508500	-3.35658800	4.70869200
C	-2.56246900	-1.00551500	4.14807100
H	-3.00275800	-0.21617400	3.52841300
H	-3.27449200	-1.83821200	4.19855100
H	-2.45687000	-0.60597000	5.16347000
C	-2.92514300	1.36378300	-3.69039500
H	-2.50442300	1.53288600	-4.68850500
H	-2.64557800	0.35034300	-3.38120200
H	-4.01694300	1.39740200	-3.78944700
C	-0.85733000	2.32265700	-2.62931100
H	-0.53781800	1.36171300	-2.21672800
H	-0.41941200	2.42969500	-3.62919000
H	-0.44085300	3.11303500	-1.99430500
C	-2.75556300	3.83457300	-3.21069000
H	-2.26623100	4.02584600	-4.17307200
H	-3.83292100	3.96588100	-3.36378200

H	-2.41760600	4.60530500	-2.50655600
H	-2.54215500	2.98615300	-0.62941600
C	6.11166500	0.24497500	-0.41156700
C	4.20146400	-0.69854200	-1.38816800
C	4.08696300	0.69862500	-1.36488800
H	7.05776700	0.36788700	0.10031700
H	3.67534600	-1.32781000	-2.09484700
H	3.25745500	1.26633300	-1.76663600
C	5.23918800	1.25935200	-0.73054800
H	5.38913300	2.31426400	-0.53366900
C	5.54935600	-1.02283800	-0.85242000
C	6.15308100	-2.24800100	-0.82677300
C	7.55159900	-2.45816200	-0.32412500
H	8.17929500	-2.86128100	-1.13069000
H	8.02518700	-1.55320900	0.05869500
H	7.55196000	-3.21650800	0.47030500
C	5.47643900	-3.49554800	-1.31362400
H	4.46123900	-3.33335500	-1.67892200
H	6.06750600	-3.94910500	-2.12105800
H	5.44371600	-4.24064600	-0.50672700

TS-2n-CuL

C	2.69356200	-1.50786900	1.45210100
C	1.52604300	-1.27830200	0.71616500
N	1.04956100	-0.00612000	0.53099500
N	1.82825400	0.95265200	1.01983000
C	4.35701200	0.08578600	-0.22695600
C	4.46460200	-1.25146200	0.17745300
C	1.25782800	2.19327000	0.90238900
O	0.04424600	2.35466400	0.59421300
C	0.79695800	-2.39652300	0.06428900
C	0.27013400	-2.28148800	-1.23473200
C	0.64468800	-3.62582400	0.73098000
C	-0.38019100	-3.35494300	-1.84196600
H	0.41207900	-1.35701500	-1.78386500
C	-0.00768400	-4.70093800	0.12410300
H	1.02640900	-3.73788200	1.74253200
C	-0.52452400	-4.57008300	-1.16595700
H	-0.75682300	-3.25056900	-2.85630300
H	-0.11232400	-5.63958400	0.66150900
H	-1.02783000	-5.40637000	-1.64244800
Cu	-0.79034100	0.54669900	0.17395000
C	-3.94988600	-0.45097300	-0.58537800
C	-3.18976100	-0.96677300	0.62212800
O	-3.79646900	-2.00275900	1.22409400
C	-1.87571600	-1.30190500	2.41348500
C	-2.91156100	-2.44267900	2.29146700
C	-3.29370800	0.74843800	-1.24568500
O	-4.14009000	1.49084200	-1.97643800
C	-1.90903000	2.28635100	-2.13269900
C	-3.37919000	2.61390600	-2.49809600
N	-2.09524000	-0.54327800	1.14946900
N	-2.05531800	1.09646900	-1.24236600
C	-0.96899000	2.04969600	-3.35460200
C	-2.00025500	-0.41133100	3.68864000
C	2.13122700	3.35777500	1.16685400
C	3.39498700	3.21527900	1.76496700
C	1.67398900	4.64180600	0.82852300
C	4.18788300	4.33447200	2.00599500
H	3.73248200	2.22898800	2.06186200
C	2.47398600	5.75705700	1.06006700
H	0.68858500	4.74654200	0.38753200

C	3.73310800	5.60631400	1.64786000
H	5.15904900	4.21738500	2.47838000
H	2.11519400	6.74586400	0.78912700
H	4.35409000	6.47796700	1.83412200
H	2.96856200	-2.53059800	1.67822400
H	3.02587100	-0.74714100	2.14556300
C	-4.04066100	-1.58490400	-1.64809500
H	-4.58145300	-1.22135200	-2.52608500
H	-3.04464100	-1.91715000	-1.95499200
H	-4.58088800	-2.43760700	-1.23026200
C	-5.38043300	-0.06856200	-0.11274400
H	-5.85551100	-0.93358200	0.35301300
H	-5.35290700	0.74911900	0.61446500
H	-5.97992400	0.25082500	-0.96646600
H	-3.52645900	-2.60211300	3.17660700
H	-2.46586200	-3.39000400	1.97582400
H	-3.75531100	3.51734200	-2.01148700
H	-3.58153800	2.67060700	-3.56750000
H	-0.86056900	-1.70772900	2.38866400
C	-0.91749400	0.68380000	3.65549100
H	-1.03931100	1.35075400	2.79781200
H	-0.96946700	1.29313500	4.56453100
H	0.08804500	0.24872500	3.60524500
C	-1.75336700	-1.30564400	4.92185900
H	-0.77708500	-1.80316500	4.86597300
H	-1.76135100	-0.69706000	5.83235700
H	-2.52050700	-2.07869200	5.04522500
C	-3.38917700	0.24621200	3.78746900
H	-3.57076700	0.92346700	2.94571400
H	-4.20087700	-0.49041400	3.81708600
H	-3.45821700	0.83961900	4.70544700
C	-1.44200900	0.85727000	-4.20609100
H	-0.78296500	0.72669200	-5.07142600
H	-1.42516400	-0.07476500	-3.63017100
H	-2.45793100	0.99671100	-4.59437300
C	0.46740600	1.79274300	-2.86223700
H	0.52736400	0.89953200	-2.23474900
H	1.13776400	1.65440200	-3.71863700
H	0.84170500	2.63787700	-2.27361400
C	-0.95777700	3.33611500	-4.20831800
H	-0.24331300	3.23196300	-5.03205500
H	-1.93306600	3.55698900	-4.65610800
H	-0.65287400	4.20622900	-3.61428600
H	-1.47395000	3.08753200	-1.52852700
C	3.68075200	-1.15220900	-2.01980100
H	3.28345300	-1.42633700	-2.98835600
H	4.63831500	0.94800700	0.36121300
H	5.11485100	-1.57388200	0.98142100
C	3.82825100	0.13186700	-1.55240100
H	3.58358300	1.03836800	-2.09251300
C	4.14107900	-2.08915400	-1.00656600
C	4.27669000	-3.43966500	-1.12906400
C	3.95290500	-4.18113400	-2.39579500
H	3.15495900	-4.91176000	-2.20667300
H	3.63665700	-3.53272900	-3.21339200
H	4.82585800	-4.75528200	-2.73251700
C	4.76936000	-4.31238400	-0.00867400
H	5.00017900	-3.76397900	0.90603700
H	4.02081800	-5.08108100	0.22611900
H	5.67439400	-4.85154600	-0.31836500

CA-2x-CuL

C	1.26000000	-1.45863800	-0.87741100
N	0.89875000	-0.28677200	-0.42611500
C	1.41782400	1.69158600	0.69870600
O	0.21386500	1.79247200	0.99915200
C	0.24965800	-2.29998600	-1.55387400
C	-0.76726600	-1.73361600	-2.34414100
C	0.32498000	-3.70327800	-1.46308100
C	-1.67919000	-2.54377300	-3.01806100
H	-0.81984500	-0.65574100	-2.44653400
C	-0.60211200	-4.51103800	-2.12221000
H	1.10108000	-4.16902000	-0.86332000
C	-1.60621000	-3.93555700	-2.90437700
H	-2.44144000	-2.08912300	-3.64520700
H	-0.53366800	-5.59146400	-2.02926900
H	-2.31922000	-4.56510700	-3.42950000
Cu	-0.93936000	0.28844100	0.14856300
C	-4.29471300	-0.26487900	0.32441300
C	-3.26818200	-1.23346500	0.88336800
O	-3.80176400	-2.42210100	1.22643500
C	-1.51423200	-2.28299200	1.80952700
C	-2.69852300	-3.26410800	1.66472900
C	-3.71049300	1.05812300	-0.14152100
O	-4.63165700	2.03492100	-0.23624200
C	-2.48898100	2.76288600	-0.95140800
C	-3.94492600	3.22841300	-0.70339600
N	-2.01180900	-1.06863000	1.10306700
N	-2.50764000	1.33942200	-0.49836900
C	-1.97305900	2.95585600	-2.40948500
C	-1.05901600	-1.99437600	3.27392200
C	2.33362300	2.82229100	1.04961000
C	2.99515300	3.57812100	0.07105900
C	2.41496700	3.20916300	2.39600200
C	3.74416700	4.69645800	0.44041100
H	2.90724900	3.31164800	-0.97835500
C	3.18107300	4.31522400	2.76170300
H	1.88223300	2.63869900	3.15123400
C	3.84709600	5.06037500	1.78479700
H	4.24476000	5.28339300	-0.32447500
H	3.25134500	4.59917600	3.80796400
H	4.43820500	5.92630800	2.06977300
N	1.89467700	0.57103600	0.06704500
C	2.66350900	-1.97235100	-0.72713000
H	2.83343400	-2.82491800	-1.38602100
H	2.81135600	-2.31990200	0.30528800
C	-5.00327400	-0.92205600	-0.89420000
H	-5.72817000	-0.22246500	-1.31962800
H	-4.28188700	-1.19705000	-1.66950000
H	-5.53399100	-1.82244200	-0.57531700
C	-5.33958600	0.00067200	1.44431900
H	-5.74522000	-0.94889300	1.80007900
H	-4.88824300	0.52864100	2.29054300
H	-6.15903000	0.60702200	1.05363900
H	-3.00953700	-3.75428800	2.58669700
H	-2.53308000	-4.01847000	0.89091500
H	-4.02687100	3.98458400	0.08071300
H	-4.47109400	3.57457100	-1.59360400
H	-0.64459200	-2.65588200	1.26115400
C	0.11321300	-0.99635800	3.25771500
H	-0.17147300	-0.05129200	2.78727400
H	0.44391100	-0.78393700	4.28163700
H	0.97375300	-1.40116900	2.71025300
C	-0.56567400	-3.31749200	3.89298800
H	0.23416200	-3.76509800	3.28956200

H	-0.16279900	-3.13489100	4.89611000
H	-1.36658600	-4.05902500	3.99326400
C	-2.20476400	-1.41528100	4.12359800
H	-2.54745300	-0.45108800	3.73149100
H	-3.06820700	-2.08915800	4.17624000
H	-1.86169700	-1.24885900	5.15159600
C	-2.78303800	2.11611400	-3.41236600
H	-2.41787600	2.29070100	-4.43132900
H	-2.69073000	1.04421400	-3.20559500
H	-3.85007700	2.37005600	-3.40230300
C	-0.48759900	2.55707400	-2.47765100
H	-0.33220600	1.53466700	-2.12175600
H	-0.11817500	2.62559400	-3.50797900
H	0.12363900	3.22435800	-1.85771000
C	-2.08441300	4.45132100	-2.77080800
H	-1.62884300	4.63427600	-3.75128200
H	-3.12352600	4.79494500	-2.82691300
H	-1.56004200	5.07727800	-2.03778700
H	-1.80341100	3.30182900	-0.29018500
C	5.19450700	-0.69172100	0.80974100
C	3.68762300	-0.86558400	-1.03014600
C	3.35581700	0.37996100	-0.18143200
H	5.98763900	-0.93355900	1.50920200
H	3.66055800	-0.63293800	-2.09701900
H	3.69290500	1.26962200	-0.71859500
C	4.20494800	0.18203900	1.05931100
H	4.07101000	0.75431200	1.96967300
C	5.07747100	-1.27288400	-0.53185000
C	5.97810400	-2.03231700	-1.19346300
C	7.32739000	-2.39034400	-0.62186700
H	8.13039900	-2.01045000	-1.26951400
H	7.49487700	-1.99464400	0.38262700
H	7.45474600	-3.48134100	-0.58335500
C	5.72731600	-2.58861300	-2.57244300
H	4.76524700	-2.28929700	-2.99498500
H	6.51645000	-2.26903800	-3.26776300
H	5.76095400	-3.68765600	-2.55619000

CA-2n-CuL

C	1.37618300	-1.51702100	-0.01416900
N	0.98991700	-0.26355500	-0.02779900
C	1.49580900	1.80044600	0.96711600
O	0.26681400	1.95160800	1.13961900
C	0.57281100	-2.51704400	-0.73996700
C	-0.11880200	-2.16214500	-1.91531000
C	0.51098000	-3.85529600	-0.30456000
C	-0.85380800	-3.11049500	-2.62290900
H	-0.04430900	-1.14592900	-2.28697400
C	-0.23734600	-4.79885300	-1.00898500
H	1.03221600	-4.16242000	0.59689600
C	-0.92244000	-4.43183300	-2.16966500
H	-1.36282500	-2.82203400	-3.53864400
H	-0.27864600	-5.82425100	-0.65212100
H	-1.49450000	-5.17099600	-2.72351500
Cu	-0.84935500	0.49281600	0.19527900
C	-4.16323700	-0.16734500	-0.29151300
C	-3.28530600	-1.00264400	0.62351700
O	-3.88560500	-2.14217000	1.01884100
C	-1.79671400	-1.83763700	2.07775500
C	-2.90803000	-2.87450900	1.80993200
C	-3.50308500	1.10361600	-0.79400300
O	-4.37944000	2.00808000	-1.26951500

C	-2.13646600	2.69812400	-1.59092900
C	-3.60565800	3.17243700	-1.67483200
N	-2.10954400	-0.76615600	1.08901800
N	-2.25265600	1.38613600	-0.88960500
C	-1.39056300	2.59572600	-2.95634400
C	-1.71364000	-1.31079400	3.54438700
C	2.41504200	2.90193400	1.39021000
C	3.27749600	3.56901100	0.50782200
C	2.30072200	3.35292000	2.71522800
C	4.02682100	4.65982600	0.95191400
H	3.35149500	3.25450300	-0.52800500
C	3.06574700	4.43004300	3.15878100
H	1.61583800	2.85275300	3.39333200
C	3.92929600	5.08677300	2.27769100
H	4.68471800	5.17577900	0.25823600
H	2.98221600	4.76096900	4.19015300
H	4.51939900	5.93161300	2.62191500
N	1.97272100	0.62833600	0.45800400
C	2.61341700	-1.90212800	0.75505300
H	2.82614300	-2.96550000	0.65639100
H	2.42077500	-1.69335600	1.81732200
C	-4.54583100	-1.01504900	-1.53894500
H	-5.16704100	-0.41873400	-2.21286700
H	-3.65322800	-1.34415400	-2.07972500
H	-5.11236100	-1.89695000	-1.23034100
C	-5.44988700	0.19667800	0.50012000
H	-5.93094100	-0.71437500	0.86210500
H	-5.21946400	0.83587900	1.35869800
H	-6.14859600	0.72736600	-0.14941600
H	-3.42054200	-3.24547000	2.69698000
H	-2.56263000	-3.71884400	1.20712200
H	-3.83437200	3.97916400	-0.97370900
H	-3.94164800	3.45520300	-2.67247100
H	-0.82010200	-2.25712700	1.82201800
C	-0.57764900	-0.27797900	3.65388900
H	-0.73926400	0.57275700	2.98698400
H	-0.50702400	0.10023300	4.68108800
H	0.39205400	-0.72551300	3.40017700
C	-1.37945000	-2.50306000	4.46351200
H	-0.45263700	-3.00016600	4.14964100
H	-1.23735400	-2.15524700	5.49340500
H	-2.17553300	-3.25592900	4.48076400
C	-3.03598800	-0.66164800	3.99186200
H	-3.27486700	0.22085600	3.38744400
H	-3.88223400	-1.35652700	3.93099600
H	-2.95972000	-0.33399400	5.03540200
C	-2.08682300	1.60918600	-3.91103400
H	-1.54461100	1.56322400	-4.86295300
H	-2.11023300	0.59546900	-3.49550000
H	-3.11784400	1.90561600	-4.13946100
C	0.05344100	2.12894600	-2.69990900
H	0.06797900	1.18336500	-2.15062100
H	0.58881500	1.99203700	-3.64716000
H	0.60353000	2.87130200	-2.10787000
C	-1.34958100	3.99880200	-3.59393700
H	-0.75594800	3.97700400	-4.51566100
H	-2.34757200	4.36651600	-3.85927900
H	-0.88875900	4.72975300	-2.91763700
H	-1.55737600	3.36867300	-0.94880800
C	4.17685100	-0.52444900	-1.99571200
C	3.38063100	0.39211100	0.03187800
C	3.84246100	-1.06617300	0.32173500
H	4.44412000	-0.61129100	-3.04333900

H	3.97547800	1.11318900	0.59330000
H	4.56621000	-1.08083800	1.14115300
C	3.56606500	0.54523500	-1.46080400
H	3.25511800	1.43577800	-1.99718700
C	4.47727900	-1.54472100	-0.99109300
C	5.19794400	-2.67545900	-1.16522600
C	5.77603600	-3.08886500	-2.49608800
H	5.45678600	-4.10952100	-2.74969900
H	5.48745800	-2.43429300	-3.32168200
H	6.87440500	-3.11290500	-2.45239700
C	5.50650800	-3.63420700	-0.04223800
H	5.20545400	-3.26664000	0.94204400
H	5.01368400	-4.60339900	-0.20703300
H	6.58497700	-3.84248500	-0.00683000

Table S1 Values of different terms used in the equation (1). Second column includes values of thermal correction to energy calculated at B3LYP/6-31G(d) level at 25°C in DCM, third column includes values of entropy calculated at B3LYP/6-31G(d) level at 25°C in DCM, fourth column includes values of total electronic energy obtained *via* single-point energy calculation at B3LYP-D3(BJ)/def2-TZVP level in DCM, and last column includes values of absolute Gibbs free energies in DCM at 25°C.

Stationary point	(U _T -U ₀)+ZPVE (a.u.)	S (cal/mol.K)	E ^{ele} (a.u.)	G (a.u.)
AD-2	0.24902700	128.323	-763.85051600	-763.66242867
FU-3	0.16248900	86.589	-310.98945100	-310.86808249
TS-1x	0.41378000	168.587	-1074.83261900	-1074.49889976
TS-1n	0.41367000	166.402	-1074.83456500	-1074.49991812
CA-1x	0.41855900	159.500	-1074.90288000	-1074.56006640
CA-1n	0.41887800	160.283	-1074.91063400	-1074.56787325
TS-2x	0.41394000	166.833	-1074.83676200	-1074.50204979
TS-2n	0.41373000	168.022	-1074.84243700	-1074.50849944
CA-2x	0.41907600	161.531	-1074.91028400	-1074.56791791
CA-2n	0.41912900	159.668	-1074.91301000	-1074.56970619
AD-2-CuL	0.72501700	216.688	-3330.69687700	-3330.07476358
TS-2x-CuL	0.88672800	252.954	-3641.68872700	-3640.92212504
TS-2n-CuL	0.88444000	248.569	-3641.69520700	-3640.92881063
CA-2x-CuL	0.89206700	251.491	-3641.75368800	-3640.98105227
CA-2n-CuL	0.89318500	246.774	-3641.75675200	-3640.98075820