

非对称笼间电子迁移异构体与电场诱导电子迁移

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Asymmetrical Inter-Cage Electron Transfer Electromers and Their Transfer Characteristics under Electric Fields

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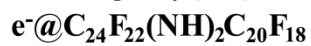
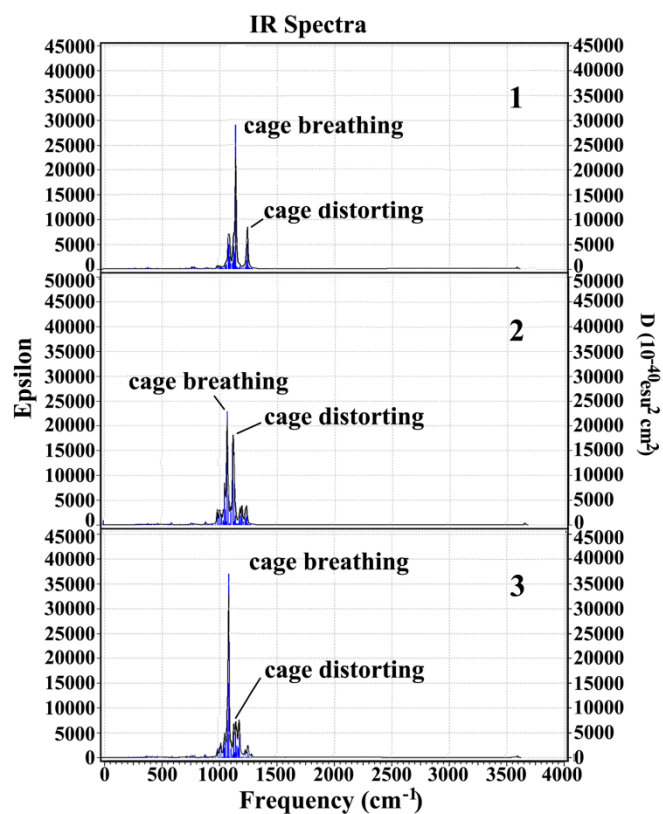
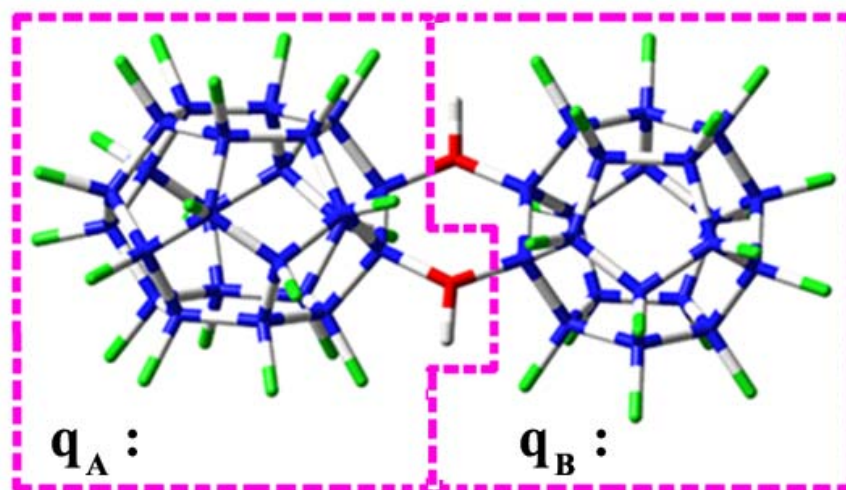


图 S1 1、2 和 3 的红外光谱



$$q_A : q_B \approx 0.581 : 0.417$$

图 S2 2 的 $C_{24}F_{22}$ 和 $C_{20}F_{18}$ 的电荷之比

B3LYP/6-31G(d) + 4s4p 方法得到的 1、2 和 3 的优化几何坐标

1

F	-4.67308900	-2.36739700	2.34318600
C	-4.18361500	-1.47395900	1.43882500
C	-2.62183200	-1.47598400	1.43563600
C	-4.66593200	-1.82141900	-0.00060800
C	-4.66383600	-0.03072900	1.77001000
C	-2.14089800	-0.03300800	1.76155400
C	-2.14167300	-1.82845000	0.00469900
F	-2.14655100	-2.36499300	2.35120100
C	-3.40273300	-2.03217500	-0.88702000
C	-5.44604700	-0.59389500	-0.55942800
F	-5.45329200	-2.93350600	0.00388500
C	-3.40019500	0.85947400	1.96761800
C	-5.44611600	0.51384200	0.53633200
F	-5.44854400	-0.02056500	2.88398300
C	-1.29809200	0.51971000	0.54039500
F	-1.40791900	-0.04148600	2.91993900
C	-1.29810100	-0.59979600	-0.56281600
F	-1.42257100	-2.97964900	0.01742800
C	-3.39990400	-0.93954700	-1.99039900
F	-3.41519200	-3.27577300	-1.44527800
C	-4.66355800	-0.04933800	-1.79298100
F	-6.71924400	-0.93830900	-0.90262900
C	-3.40281100	1.95207300	0.86424900
F	-3.40284400	1.42384700	3.20892300
C	-4.66587800	1.74134400	-0.02236500
F	-6.71936100	0.85828600	0.87932700
C	-2.14157900	1.74836100	-0.02729600
C	-2.14060600	-0.04709900	-1.78416600
F	-3.40237700	-1.50395900	-3.23169800
C	-4.18335000	1.39387900	-1.46171800
F	-5.44809100	-0.05948500	-2.90708000
F	-3.41536200	3.19567300	1.42247600
F	-5.45321700	2.85344500	-0.02698400
C	-2.62156100	1.39588100	-1.45832300
F	-1.42267900	2.89964300	-0.03996500
F	-1.40721300	-0.03882400	-2.94221400
F	-4.67268300	2.28732200	-2.36615500
F	-2.14615100	2.28487300	-2.37382300
N	-0.00633300	0.93525100	0.98819200
N	-0.00631400	-1.01522400	-1.01003700
H	0.02999400	-1.15224400	-2.01029900
C	1.28761300	-0.66024700	-0.47633500
C	1.28758900	0.58023200	0.45390800
C	1.98093500	-1.81732300	0.31929300
C	2.24950200	-0.35380700	-1.70683900
C	1.98052200	1.73739100	-0.34190200
C	2.24983600	0.27379900	1.68407300

C	3.10245600	-2.41564000	-0.54481900
C	2.64369400	-1.23098000	1.60604400
F	1.08758800	-2.79077000	0.67255500
C	2.64322800	1.15113000	-1.62887700
C	3.34802200	-1.46494000	-1.75685600
F	1.53453500	-0.49520400	-2.89570100
C	3.10215600	2.33585900	0.52201400
F	1.08682700	2.71030500	-0.69547900
C	3.34819300	1.38512700	1.73384800
F	1.53515800	0.41514000	2.87332900
C	4.39450700	-2.46225500	0.28856000
F	2.76280200	-3.66810500	-0.98530800
C	4.15772500	-1.63472000	1.59325900
F	2.07257900	-1.85921300	2.69307700
C	4.15722300	1.55522400	-1.61624900
F	2.07195200	1.77909200	-2.71578800
C	4.86019700	-1.06181900	-1.74340600
F	3.13794000	-2.19907300	-2.90641300
C	4.39403800	2.38280100	-0.31150300
F	2.76212300	3.58828500	0.96248200
C	4.86030200	0.98230000	1.72030000
F	3.13791000	2.11932600	2.88352300
C	5.51239100	-1.77799700	-0.51611800
F	4.73213800	-3.75391200	0.59530000
C	5.26784100	-0.52834700	1.65070900
F	4.36391200	-2.47191300	2.66751200
C	5.26754200	0.44903100	-1.67380700
F	4.36312600	2.39231800	-2.69045600
F	5.42898600	-1.58159800	-2.88629900
C	5.51216300	1.69858500	0.49303300
F	4.73159200	3.67439100	-0.61837300
F	5.42918500	1.50231400	2.86325800
C	6.15800000	-0.70420200	0.37484000
F	6.44341600	-2.69143100	-0.93619100
F	6.04985000	-0.79280500	2.75328500
C	6.15793400	0.62500800	-0.39798600
F	6.04928700	0.71335300	-2.77641300
F	6.44297700	2.61244900	0.91285800
F	7.43218000	-1.06422100	0.72925300
F	7.43192600	0.98509900	-0.75274200
H	0.03009000	1.06806200	1.98905500

2

F	-4.67066753	-2.35962950	2.35345490
C	-4.18238381	-1.46606741	1.44195750
C	-2.62355524	-1.46761944	1.43838357
C	-4.66357049	-1.81832423	0.00619171
C	-4.66153004	-0.02390662	1.76719588
C	-2.14390974	-0.02697899	1.75913393
C	-2.14405526	-1.82518885	0.01105715

F	-2.14187481	-2.35605526	2.35872839
C	-3.40272456	-2.03204619	-0.87836504
C	-5.44201247	-0.59489650	-0.55636561
F	-5.45169345	-2.93523658	0.01474704
C	-3.40009225	0.86543503	1.96132856
C	-5.44199332	0.51513371	0.53324302
F	-5.44736732	-0.00901497	2.88581216
C	-1.30457136	0.51970676	0.53613226
F	-1.40145246	-0.02934845	2.91849401
C	-1.30456558	-0.60033061	-0.55852735
F	-1.41834258	-2.97792207	0.02782141
C	-3.39992928	-0.94563498	-1.98408220
F	-3.41233649	-3.28232805	-1.43303724
C	-4.66121527	-0.05602574	-1.79017922
F	-6.71937221	-0.94212254	-0.89951121
C	-3.40246151	1.95185063	0.85560965
F	-3.39955450	1.43675964	3.20478062
C	-4.66319307	1.73839777	-0.02917459
F	-6.71934131	0.86262820	0.87616058
C	-2.14368890	1.74471422	-0.03360010
C	-2.14359852	-0.05348611	-1.78166134
F	-3.39928664	-1.51696213	-3.22753265
C	-4.18182685	1.38603560	-1.46485743
F	-5.44685545	-0.07075594	-2.90893578
F	-3.41189834	3.20213590	1.41027737
F	-5.45107929	2.85547609	-0.03786928
C	-2.62300259	1.38724921	-1.46100592
F	-1.41765378	2.89725226	-0.05026191
F	-1.40093272	-0.05126939	-2.94088654
F	-4.66975619	2.27969861	-2.37644535
F	-2.14096070	2.27558222	-2.38126041
N	-0.00744344	0.93675390	0.98511408
N	-0.00741264	-1.01745883	-1.00739912
H	0.02068788	-1.16839145	-2.00574583
C	1.28241780	-0.65994485	-0.47869808
C	1.28235772	0.57946058	0.45625938
C	1.97711144	-1.82212646	0.31500886
C	2.24285614	-0.34977885	-1.71079989
C	1.97653608	1.74184226	-0.33755607
C	2.24306782	0.26959044	1.68820223
C	3.09959262	-2.41937124	-0.55235151
C	2.63920828	-1.23859973	1.60353866
F	1.08911163	-2.79616681	0.66741512
C	2.63857025	1.15852317	-1.62620569
C	3.34481489	-1.46249375	-1.76227334
F	1.53624186	-0.48644772	-2.89796451
C	3.09898374	2.33943348	0.52960524
F	1.08811852	2.71558613	-0.68975327
C	3.34470370	1.38263143	1.73948532
F	1.53655311	0.40610092	2.87544497

C	4.39475562	-2.46903338	0.28020335
F	2.76317056	-3.66776437	-0.99832921
C	4.15698416	-1.64239386	1.58768271
F	2.07605658	-1.86800436	2.68886181
C	4.15622558	1.56277254	-1.61061924
F	2.07503371	1.78775608	-2.71142802
C	4.86030612	-1.05846124	-1.74724123
F	3.14066822	-2.18999440	-2.91238223
C	4.39398273	2.38948410	-0.30318125
F	2.76225739	3.58772580	0.97563552
C	4.86031379	0.97905008	1.72418335
F	3.14053174	2.11006741	2.88963072
C	5.51519388	-1.78072908	-0.52210538
F	4.73301504	-3.75771685	0.58559170
C	5.26724706	-0.53414116	1.64657774
F	4.36580224	-2.47680196	2.65826506
C	5.26680591	0.45485078	-1.66971100
F	4.36460351	2.39724132	-2.68124062
F	5.42758117	-1.56891314	-2.88985829
C	5.51476768	1.70151381	0.49892919
F	4.73180188	3.67826913	-0.60862832
F	5.42764462	1.48966806	2.86669848
C	6.16215042	-0.70695238	0.37198526
F	6.44453459	-2.68946381	-0.94694935
F	6.04609968	-0.79999715	2.74682514
C	6.16188404	0.62792995	-0.39527766
F	6.04538323	0.72093710	-2.77009742
F	6.44391328	2.61052612	0.92360594
F	7.43255207	-1.06668049	0.72864664
F	7.43211459	0.98803629	-0.75216632
H	0.02069999	1.08775665	1.98345060

3

F	4.67301400	-2.36599300	2.34932300
C	4.18546500	-1.46680700	1.43608500
C	2.62916200	-1.46802600	1.43306400
C	4.66508100	-1.81505100	0.00214100
C	4.66362700	-0.02797800	1.76378600
C	2.15104700	-0.03010800	1.75558500
C	2.14955000	-1.82128500	0.00653000
F	2.14245700	-2.36033100	2.35314400
C	3.40674800	-2.02658400	-0.88154200
C	5.44250400	-0.59268800	-0.55625300
F	5.45423300	-2.93703300	0.00807100
C	3.40494000	0.86012900	1.95950600
C	5.44254100	0.51237700	0.53329700
F	5.45052100	-0.01538500	2.88747400
C	1.31120600	0.51858600	0.53625000
F	1.40153100	-0.03282700	2.91715700
C	1.31119500	-0.59906600	-0.55878700

F	1.41777100	-2.97555600	0.02232800
C	3.40477100	-0.94051800	-1.98226100
F	3.41224900	-3.28028500	-1.43931300
C	4.66343900	-0.05235700	-1.78665800
F	6.72403400	-0.94134000	-0.90165100
C	3.40674800	1.94618200	0.85879800
F	3.40056700	1.43007800	3.20857900
C	4.66500400	1.73471600	-0.02501200
F	6.72409400	0.86108800	0.87855100
C	2.14944400	1.74083400	-0.02914300
C	2.15085700	-0.05034000	-1.77821100
F	3.40030100	-1.51047000	-3.23132500
C	4.18525100	1.38646800	-1.45889000
F	5.45021600	-0.06489300	-2.91042100
F	3.41225100	3.19989100	1.41655700
F	5.45410600	2.85673300	-0.03100700
C	2.62893900	1.38761000	-1.45571900
F	1.41764900	2.89509200	-0.04483500
F	1.40118900	-0.04766400	-2.93966000
F	4.67264500	2.28565500	-2.37220400
F	2.14210100	2.27988900	-2.37574700
N	0.00774200	0.93247800	0.99115000
N	0.00770200	-1.01307000	-1.01345300
H	-0.01343200	-1.14711700	-2.01424300
C	-1.27759700	-0.65942900	-0.48405300
C	-1.27752900	0.57903900	0.46150000
C	-1.97566700	-1.82718200	0.30748900
C	-2.24177000	-0.34342500	-1.71392200
C	-1.97527100	1.74691600	-0.33013300
C	-2.24192300	0.26321600	1.69124800
C	-3.10150900	-2.42054000	-0.56210100
C	-2.63864400	-1.24841200	1.60092600
F	-1.09518300	-2.80353300	0.65573600
C	-2.63820900	1.16827400	-1.62365400
C	-3.34699700	-1.45793700	-1.77002500
F	-1.54643400	-0.47318400	-2.90105400
C	-3.10110200	2.34050000	0.53932500
F	-1.09456600	2.72309700	-0.67828400
C	-3.34693000	1.37795200	1.74721700
F	-1.54671800	0.39282200	2.87848300
C	-4.39877200	-2.47357200	0.27069800
F	-2.77016900	-3.66446700	-1.01377400
C	-4.16013400	-1.65111700	1.58291700
F	-2.08242200	-1.87961700	2.68196400
C	-4.15962100	1.57128200	-1.60582500
F	-2.08173500	1.79936200	-2.70462800
C	-4.86551600	-1.05381100	-1.75327500
F	-3.14629300	-2.17783000	-2.91946300
C	-4.39825400	2.39378600	-0.29363600
F	-2.76957400	3.58436400	0.99102700

C	-4.86552600	0.97412000	1.73028300
F	-3.14622900	2.09780300	2.89668000
C	-5.52132400	-1.78156200	-0.52878700
F	-4.73810500	-3.75965500	0.57204500
C	-5.27287500	-0.54142300	1.64679600
F	-4.37068600	-2.48643200	2.64692300
C	-5.27257800	0.46181000	-1.66983700
F	-4.36987600	2.40663900	-2.66985600
F	-5.43226600	-1.55794800	-2.89351900
C	-5.52104000	1.70200100	0.50571500
F	-4.73729600	3.67993500	-0.59502500
F	-5.43230900	1.47837100	2.87046000
C	-6.16932400	-0.70959700	0.36973900
F	-6.44895500	-2.68568700	-0.95703500
F	-6.04946000	-0.81056300	2.74223500
C	-6.16914600	0.63016300	-0.39288600
F	-6.04897900	0.73109800	-2.76536900
F	-6.44854100	2.60631200	0.93385100
F	-7.43649000	-1.06945800	0.72558100
F	-7.43619900	0.99027400	-0.74887900
H	-0.01343300	1.06559300	1.99206900