

**Modelling photophysical properties of metal-organic frameworks:
A Density Functional Theory based approach**

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SUPPORTING INFORMATION

Complete Gaussian Reference

Gaussian 09, Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Scalmani, G.; Barone, V.; Mennucci, B.; Petersson, G. A.; Nakatsuji, H.; Caricato, M.; Li, X.; Hratchian, H. P.; Izmaylov, A. F.; Bloino, J.; Zheng, G.; Sonnenberg, J. L.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Vreven, T.; Montgomery, J. A., Jr.; Peralta, J. E.; Ogliaro, F.; Bearpark, M.; Heyd, J. J.; Brothers, E.; Kudin, K. N.; Staroverov, V. N.; Kobayashi, R.; Normand, J.; Raghavachari, K.; Rendell, A.; Burant, J. C.; Iyengar, S. S.; Tomasi, J.; Cossi, M.; Rega, N.; Millam, J. M.; Klene, M.; Knox, J. E.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Martin, R. L.; Morokuma, K.; Zakrzewski, V. G.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Dapprich, S.; Daniels, A. D.; Farkas, Ö.; Foresman, J. B.; Ortiz, J. V.; Cioslowski, J.; Fox, D. J. Gaussian, Inc., Wallingford CT, 2009.

Table S1. Vertical excitation energies and associated oscillator strengths computed at PBE0 for Zn[DMPMB].

Transition	Wavelength (nm)	Oscillator Strength (a.u.)	Character
1	264	0.235	$\pi - \pi^*$ biphenyl
2	266	2.995	
3	267	1.020	$\pi - \pi^*$ pyrazole
4	266	0.128	

Table S2. Vertical excitation energies and associated oscillator strengths computed at CAM-B3LYP for Zn[DMPMB].

Transition	Wavelength (nm)	Oscillator Strength (a.u.)	Character
1	259	0.188	$\pi - \pi^*$ biphenyl
2	254	3.276	
3	252	0.917	$\pi - \pi^*$ pyrazole
4	248	0.259	

Table S3. Vertical excitation energies and associated oscillator strengths computed at PBE0 for Cd[DMPMB].

Transition	Wavelength (nm)	Oscillator Strength (a.u.)	Character
1	269	0.195	$\pi - \pi^*$ biphenyl
2	269	2.995	
3	270	0.998	$\pi - \pi^*$ pyrazole
4	270	0.224	

Table S4. Vertical excitation energies and associated oscillator strengths computed at PBE0 for H₂DMPMB ligand.

Transition	Wavelength (nm)	Oscillator Strength (a.u.)	Character
1	259	0.748	$\pi - \pi^*$
2	252	0.001	
3	248	0.016	
4	238	0.000	
5	237	0.010	

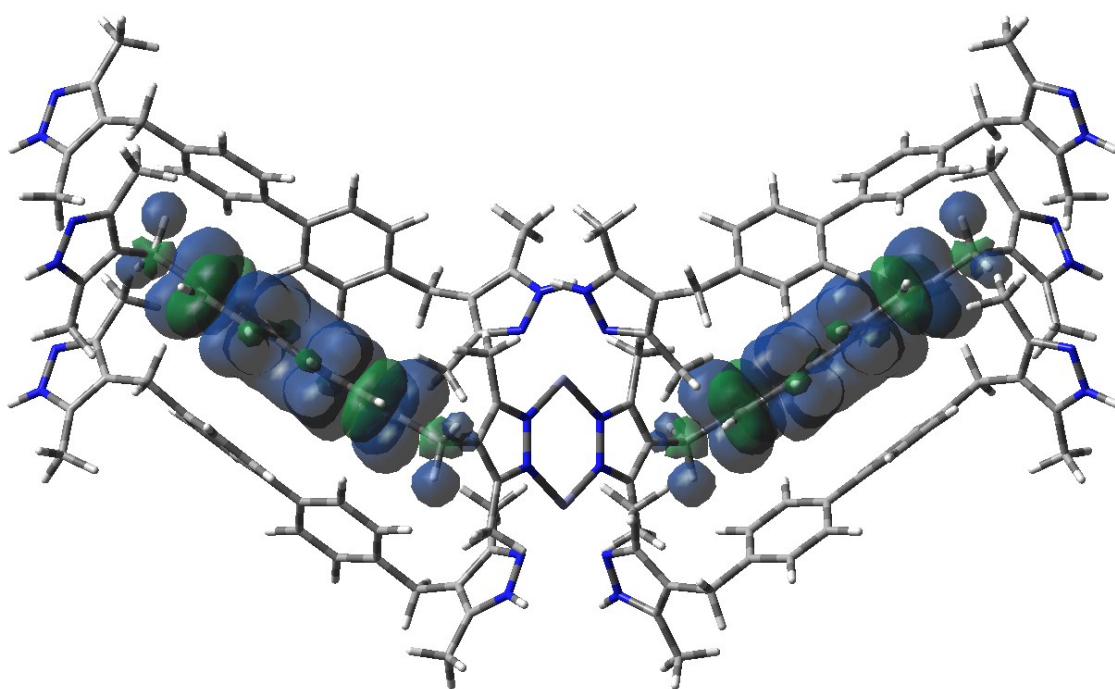


Figure S1. Spin density difference plot ($\rho_\alpha - \rho_\beta$) computed for the first triplet state of the Zn[DMPMB] cluster.

Table S5. XYZ coordinates (in Å) for the Zn[DMPMB] model used.

Atom	X	Y	Z
C	34.26357000	-0.80854000	-8.77979000
C	34.14393000	-4.33163000	-12.98180000
C	33.07611000	-1.50705000	-8.21890000
C	49.43681000	-3.58083000	-8.08389000
C	50.12946000	1.74855000	-9.17994000
C	50.44640000	-3.44301000	-7.00024000
C	35.01445000	1.55843000	-15.72240000
C	49.02460000	2.16225000	-10.08586000
C	33.82699000	0.85993000	-15.16150000
C	50.18769000	-1.21386000	-15.02649000
C	51.19728000	-1.07604000	-13.94285000
C	35.42667000	-4.18465000	-13.72042000
C	31.78201000	-0.97525000	-8.33988000
C	51.23638000	2.57865000	-8.93954000
C	33.06814000	-5.06360000	-13.51003000
C	48.11158000	-3.14717000	-7.91704000
C	35.55767000	-1.34034000	-8.65881000
C	51.77163000	-3.87667000	-7.16709000
C	32.53289000	1.39172000	-15.28249000
C	48.86245000	-0.78020000	-14.85965000
C	36.30855000	1.02663000	-15.60141000
C	52.52251000	-1.50970000	-14.10969000
C	47.91767000	1.33214000	-10.32626000
C	36.50246000	-3.45268000	-13.19219000
C	30.66493000	-1.65139000	-7.85602000
C	52.29301000	2.17258000	-8.12850000
C	31.85134000	-5.16244000	-12.84014000
C	47.15467000	-3.31841000	-8.91411000
C	36.67475000	-0.66420000	-9.14267000
C	52.72854000	-3.70544000	-6.17001000
C	31.41581000	0.71558000	-14.79863000
C	47.90554000	-0.95143000	-15.85672000
C	37.42563000	1.70277000	-16.08528000
C	53.47942000	-1.33846000	-13.11262000
C	46.86104000	1.73821000	-11.13730000
C	37.71926000	-3.35385000	-13.86209000
C	36.55404000	0.57548000	-9.77369000
C	31.64986000	-4.53708000	-11.60810000
C	30.78564000	-2.89107000	-7.22500000
C	47.47494000	-3.92901000	-10.12827000
C	52.29492000	0.91814000	-7.51536000
C	52.40826000	-3.09484000	-4.95586000
C	37.30492000	2.94246000	-16.71630000
C	46.85913000	2.99266000	-11.75045000
C	31.53652000	-0.52410000	-14.16760000
C	48.22582000	-1.56203000	-17.07087000
C	53.15914000	-0.72786000	-11.89847000
C	37.92073000	-3.97921000	-15.09412000
C	35.26627000	1.09580000	-9.93043000
C	32.72667000	-3.83613000	-11.05781000
C	32.07341000	-3.41139000	-7.06826000
C	48.80008000	-4.33152000	-10.31703000
C	51.18075000	0.09940000	-7.72015000
C	51.08313000	-2.69232000	-4.76710000
C	36.01715000	3.46277000	-16.87304000
C	47.97330000	3.81139000	-11.54566000
C	32.82430000	-1.04441000	-14.01086000
C	49.55096000	-1.96455000	-17.25964000
C	51.83401000	-0.32534000	-11.70970000
C	36.84393000	-4.68015000	-15.64441000
C	34.15089000	0.42262000	-9.44921000
C	33.94122000	-3.73706000	-11.72404000
C	33.18879000	-2.73821000	-7.54948000
C	49.75602000	-4.16094000	-9.32411000

C	50.12563000	0.50291000	-8.52806000
C	50.12719000	-2.86291000	-5.76002000
C	34.90177000	2.78959000	-16.39181000
C	49.02842000	3.40789000	-10.73774000
C	33.93967000	-0.37124000	-14.49209000
C	50.50690000	-1.79396000	-16.26672000
C	50.87806000	-0.49593000	-12.70262000
C	35.62938000	-4.77923000	-14.97818000
C	37.74988000	1.38921000	-10.23477000
C	30.31428000	-4.54182000	-10.88633000
C	29.58981000	-3.70480000	-6.76392000
C	46.44553000	-4.21810000	-11.20600000
C	53.46408000	0.39825000	-6.69832000
C	53.43768000	-2.80574000	-3.87813000
C	38.50076000	3.75618000	-17.17737000
C	45.68997000	3.51255000	-12.56748000
C	30.34068000	-1.33783000	-13.70653000
C	47.19641000	-1.85113000	-18.14861000
C	54.18855000	-0.43877000	-10.82073000
C	39.25632000	-3.97447000	-15.81589000
C	39.02811000	0.63780000	-10.42788000
C	29.35130000	-5.61534000	-11.28131000
C	28.31157000	-2.95339000	-6.57082000
C	45.18172000	-3.42124000	-11.14619000
C	54.41264000	1.42632000	-6.17005000
C	54.70149000	-3.60260000	-3.93794000
C	39.77900000	3.00477000	-17.37048000
C	44.74141000	2.48447000	-13.09576000
C	29.06245000	-0.58642000	-13.51342000
C	45.93260000	-1.05427000	-18.08880000
C	55.45237000	-1.23563000	-10.88054000
C	40.21931000	-2.90095000	-15.42092000
C	39.95390000	0.26769000	-9.44665000
C	28.49067000	-5.62246000	-12.38410000
C	27.38578000	-2.58328000	-7.55205000
C	44.06275000	-3.66007000	-10.34135000
C	55.46644000	2.04238000	-6.85333000
C	55.82046000	-3.36377000	-4.74278000
C	40.70478000	2.63466000	-16.38925000
C	43.68761000	1.86842000	-12.41248000
C	28.13666000	-0.21631000	-14.49465000
C	44.81363000	-1.29310000	-17.28396000
C	56.57133000	-0.99680000	-11.68538000
C	41.07993000	-2.89382000	-14.31812000
C	27.77998000	-2.44426000	-5.38066000
C	55.02710000	-4.76103000	-3.22360000
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C	29.11973000	-6.84300000	-10.65084000
C	55.77798000	-2.39406000	-10.16621000
C	44.85611000	-2.26281000	-11.86053000
C	39.55971000	0.12867000	-11.61803000
C	44.71582000	1.90612000	-14.36977000
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C	27.39926000	-2.91495000	-9.00654000
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H	39.71769000	2.74036000	-14.48915000
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H	40.70512000	0.04533000	-7.43956000
H	27.64966000	-4.88029000	-14.22368000
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H	56.94973000	1.08169000	-12.04980000
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H	55.52607548	-3.32138960	-8.29386829
H	45.10802768	-1.33556400	-13.73290582
H	39.52562465	-0.44596905	-13.64230251
H	45.47076613	1.43065301	-16.27582355
H	40.04521810	-0.09392985	-17.38184461
H	45.99120002	1.78203402	-20.01398642
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H	29.86550000	-4.22776000	-5.83891000
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H	46.92710000	-4.09210000	-12.18446000
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H	47.67798000	-1.72513000	-19.12706000
H	37.91496000	2.18719000	-9.49316000
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H	29.42473000	-4.50278000	-7.50553000
H	46.19384000	-5.28914000	-11.14668000
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H	45.13095000	4.22056000	-11.93487000
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H	39.72872000	-4.95554000	-15.64759000
N	26.62313000	-1.80666000	-5.64198000

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N	56.25175000	-5.18489000	-3.58922000
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N	41.37817000	-0.98207000	-15.36186000
N	26.38486000	-1.88488000	-6.98397000
N	56.06200000	2.93913000	-6.04496000
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N	43.14588000	-2.69675000	-10.55031000
N	40.95482000	-0.43071000	-10.01472000
N	56.73733000	-4.32709000	-4.53382000
N	27.13574000	0.48209000	-13.92658000
N	43.89676000	-0.32978000	-17.49291000
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N	43.09206000	0.97166000	-13.22085000
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Zn	42.67517000	0.40589000	-16.05963000
Zn	42.29974000	-0.77760000	-12.58832000
H	26.35155251	0.87629875	-14.40579753
H	27.14125803	-7.05192049	-13.10799093
H	25.60067028	-1.49067141	-7.46318402
H	57.62292829	-4.40162899	-4.99225169
H	58.37380377	-2.03465861	-11.93487047
H	56.83324320	3.52658998	-6.29006142
H	41.73900749	-0.82491875	-9.53550247
H	42.26028264	-2.62221121	-10.09187649
H	42.05172510	1.40500596	-18.97263968
H	43.90965712	1.33292190	-18.79627634
H	29.92817792	-0.84124951	-10.94743657
H	29.45365480	0.81484315	-10.65545786
H	30.83953325	-7.28813512	-9.52248294
H	29.44207104	-6.84641473	-8.57114225
H	29.17739978	-3.20810828	-4.00486758
H	28.70262877	-1.55210631	-3.71277749
H	37.95528866	-0.09413659	-12.96162235
H	39.05112834	1.21013109	-13.35032260
H	38.73103359	-1.22751565	-17.17943670
H	40.12800232	-1.67031038	-18.13100270
H	38.70616874	2.27283311	-19.90422240
H	39.80200805	3.57710115	-20.29292247
H	46.53828628	-2.12890937	-13.11806427
H	46.02120253	-0.60660544	-12.43375310
H	46.64548857	2.12071744	-15.18179205
H	45.43169427	3.14024154	-15.91687074
H	47.42134125	0.98804844	-19.39969852
H	46.50762016	0.25974675	-20.69883557
H	54.09584351	-2.52791872	-8.90860982
H	54.61279958	-4.05022090	-9.59302138
H	52.50860075	1.78841208	-4.08436779
H	53.72350288	0.77123398	-3.34787053
H	53.34497359	-4.89489082	-1.96599478
H	53.86192937	-6.41719124	-2.65041047

Table S6. XYZ coordinates (in Å) for the Cd[DMPMB]model used.

Atom	X	Y	Z
C	33.06372000	9.99327000	-8.09739000
C	32.72777000	10.76467000	-13.52309000
C	32.04614000	8.90924000	-8.15106000
C	48.36286000	9.17817000	-10.19658000
C	48.65158000	13.76759000	-7.19658000
C	49.39580000	8.51789000	-9.35364000
C	33.00114000	17.09840000	-11.31237000
C	47.51176000	14.68229000	-7.47514000
C	31.98356000	16.01437000	-11.36603000
C	48.30028000	16.28330000	-13.41155000
C	49.33322000	15.62302000	-12.56861000
C	33.85223000	11.59428000	-14.03380000
C	30.74654000	9.08780000	-7.65022000
C	49.69879000	14.13035000	-6.33434000
C	31.68110000	10.34114000	-14.35783000
C	47.06273000	9.41751000	-9.72324000
C	34.36332000	9.81470000	-8.59823000
C	50.69593000	8.27855000	-9.82698000
C	30.68396000	16.19293000	-10.86519000
C	47.00014000	16.52264000	-12.93821000
C	34.30074000	16.91983000	-11.81321000
C	50.63335000	15.38368000	-13.04195000
C	46.46456000	14.31953000	-8.33738000
C	34.89890000	12.01781000	-13.19906000
C	29.78343000	8.08423000	-7.73823000
C	50.78531000	13.28765000	-6.10672000
C	30.60855000	9.59810000	-13.86792000
C	46.08565000	9.99967000	-10.52877000
C	35.32642000	10.81827000	-8.51022000
C	51.67301000	7.69639000	-9.02145000
C	29.72085000	15.18936000	-10.95320000
C	46.02307000	17.10480000	-13.74374000
C	35.26384000	17.92340000	-11.72519000
C	51.61042000	14.80152000	-12.23642000
C	45.37804000	15.16223000	-8.56500000
C	35.97145000	12.76085000	-13.68897000
C	35.03794000	12.04814000	-7.91646000
C	30.52936000	9.24349000	-12.52022000
C	30.07191000	6.85437000	-8.33199000
C	46.36004000	10.36961000	-11.84642000
C	50.87859000	12.04247000	-6.73054000
C	51.39862000	7.32646000	-7.70380000
C	34.97536000	19.15327000	-11.13143000
C	45.28476000	16.40741000	-7.94117000
C	30.00933000	13.95950000	-11.54696000
C	46.29746000	17.47474000	-15.06139000
C	51.33604000	14.43159000	-10.91877000
C	36.05065000	13.11546000	-15.03668000
C	33.74034000	12.24062000	-7.43234000
C	31.57734000	9.64523000	-11.68623000
C	31.36952000	6.66189000	-8.81611000
C	47.65786000	10.15198000	-12.31916000
C	49.83038000	11.66587000	-7.57591000
C	50.10079000	7.54409000	-7.23105000
C	33.67776000	19.34575000	-10.64731000
C	46.33296000	16.78401000	-7.09581000
C	31.30694000	13.76702000	-12.03109000
C	47.59528000	17.25711000	-15.53414000
C	50.03821000	14.64922000	-10.44603000
C	35.00266000	12.71371000	-15.87066000
C	32.77838000	11.24511000	-7.52307000
C	32.64853000	10.38071000	-12.17229000
C	32.33148000	7.65739000	-8.72538000

C	48.63365000	9.57716000	-11.51789000
C	48.74537000	12.50071000	-7.80040000
C	49.12500000	8.11890000	-8.03233000
C	32.71580000	18.35024000	-10.73804000
C	47.41798000	15.94917000	-6.87132000
C	32.26889000	14.76252000	-11.94036000
C	48.57107000	16.68229000	-14.73286000
C	49.06242000	15.22403000	-11.24730000
C	33.93148000	11.97823000	-15.38461000
C	36.06198000	13.15540000	-7.74134000
C	29.35849000	8.48576000	-11.92000000
C	29.04787000	5.74710000	-8.50711000
C	45.32110000	10.95389000	-12.78694000
C	52.06436000	11.10865000	-6.56536000
C	52.43756000	6.74217000	-6.76328000
C	35.99940000	20.26053000	-10.95632000
C	44.09899000	17.34123000	-8.10636000
C	28.98529000	12.85223000	-11.72208000
C	45.25852000	18.05902000	-16.00191000
C	52.37498000	13.84730000	-9.97825000
C	37.22152000	13.87319000	-15.63690000
C	37.37251000	12.96500000	-8.43404000
C	28.36180000	7.92906000	-12.88450000
C	27.73735000	5.93750000	-7.81441000
C	44.00895000	11.32937000	-12.17799000
C	53.06268000	11.48026000	-5.51711000
C	53.74971000	6.36669000	-7.37223000
C	37.30993000	20.07014000	-11.64902000
C	43.10067000	16.96962000	-9.15461000
C	27.67476000	13.04263000	-11.02938000
C	43.94636000	18.43451000	-15.39296000
C	53.68713000	13.47182000	-10.58720000
C	38.21820000	14.42989000	-14.67240000
C	38.43531000	12.14264000	-8.04111000
C	27.35373000	8.62111000	-13.56647000
C	26.67454000	6.75986000	-8.20734000
C	42.96089000	10.47594000	-11.81264000
C	54.05599000	12.46400000	-5.59341000
C	54.79776000	7.22013000	-7.73757000
C	38.37273000	19.24777000	-11.25609000
C	42.10736000	15.98588000	-9.07831000
C	26.61196000	13.86499000	-11.42231000
C	42.89831000	17.58107000	-15.02761000
C	54.73518000	14.32525000	-10.95255000
C	39.22627000	13.73783000	-13.99042000
C	27.29961000	5.35097000	-6.61930000
C	54.20388000	5.08831000	-7.72349000
C	27.23702000	12.45610000	-9.83427000
C	53.20702000	10.93942000	-4.23237000
C	28.23388000	6.60499000	-13.32539000
C	54.14130000	12.19344000	-10.93846000
C	43.55478000	12.60776000	-11.82673000
C	37.81025000	13.55153000	-9.62915000
C	42.95632000	17.51046000	-10.43935000
C	38.34612000	15.75396000	-14.23150000
C	43.49220000	19.71288000	-15.04170000
C	37.74767000	20.65666000	-12.84412000
C	38.55676000	11.28101000	-6.82769000
C	26.98715000	10.06631000	-13.48543000
C	26.55310000	7.62150000	-9.42076000
C	42.86010000	8.99405000	-11.96565000
C	54.40193000	13.36232000	-6.73486000
C	54.89856000	8.70201000	-7.58456000
C	38.49417000	18.38614000	-10.04267000
C	41.76142000	15.08756000	-7.93686000
C	26.49052000	14.72663000	-12.63573000
C	42.79752000	16.09919000	-15.18063000

C	54.83598000	15.80714000	-10.79953000
C	39.59285000	12.29264000	-14.07146000
C	28.00878000	4.36745000	-5.74908000
C	53.51493000	3.77517000	-7.55451000
C	27.94620000	11.47258000	-8.96405000
C	52.42866000	9.83915000	-3.59122000
C	29.03247000	5.40861000	-12.92734000
C	53.45235000	10.88030000	-10.76948000
C	44.24372000	13.92089000	-11.99571000
C	37.10108000	14.53505000	-10.49937000
C	43.73469000	18.61073000	-11.08050000
C	37.54753000	16.95034000	-14.62955000
C	44.18114000	21.02602000	-15.21068000
C	37.03850000	21.64018000	-13.71434000
Cd	40.64283000	17.58486000	-12.76649000
Cd	40.67412000	14.03230000	-11.15900000
H	30.45959000	10.02711000	-7.18399000
H	46.78646000	9.14357000	-8.70803000
H	34.65026000	8.87540000	-9.06446000
H	50.97219000	8.55250000	-10.84218000
H	46.47685000	13.35867000	-8.84590000
H	34.89729000	11.76543000	-12.14157000
H	30.39701000	17.13224000	-10.39896000
H	49.68649000	15.09121000	-5.82582000
H	31.68271000	10.59352000	-15.41533000
H	46.72388000	16.24870000	-11.92301000
H	34.58768000	15.98053000	-12.27943000
H	50.90961000	15.65763000	-14.05716000
H	28.78646000	8.26576000	-7.34527000
H	51.57925000	13.60974000	-5.43797000
H	29.81442000	9.29676000	-14.54606000
H	45.08886000	10.16045000	-10.12642000
H	36.32339000	10.63675000	-8.90318000
H	52.66980000	7.53561000	-9.42379000
H	28.72388000	15.37089000	-10.56024000
H	45.02628000	17.26558000	-13.34140000
H	36.26081000	17.74188000	-12.11815000
H	52.60721000	14.64074000	-12.63876000
H	44.58410000	14.84014000	-9.23375000
H	36.76558000	13.06219000	-13.01083000
H	33.47708000	13.19051000	-6.97278000
H	31.55399000	9.37762000	-10.63237000
H	31.63277000	5.71200000	-9.27567000
H	47.91024000	10.43756000	-13.33775000
H	49.86462000	10.69800000	-8.07073000
H	49.84842000	7.25850000	-6.21246000
H	33.41450000	20.29564000	-10.18775000
H	46.29873000	17.75187000	-6.60099000
H	31.57019000	12.81713000	-12.49064000
H	47.84766000	17.54270000	-16.55272000
H	49.78584000	14.36363000	-9.42744000
H	35.02601000	12.98133000	-16.92452000
H	31.79439000	11.46157000	-7.11799000
H	49.61703000	9.43014000	-11.95439000
H	47.97260000	12.14637000	-8.47602000
H	33.42191000	10.66562000	-11.46525000
H	48.14162000	8.26592000	-7.59583000
H	33.31547000	7.44093000	-9.13046000
H	31.73181000	18.56670000	-10.33296000
H	48.19075000	16.30351000	-6.19570000
H	33.15809000	11.69333000	-16.09164000
H	49.55445000	16.53527000	-15.16936000
H	48.07904000	15.37105000	-10.81080000
H	33.25288000	14.54606000	-12.34544000
H	39.50437000	10.73103000	-6.81916000
H	41.92070000	8.61080000	-11.55191000
H	55.21329000	14.05036000	-6.47252000

H	55.83796000	9.08526000	-7.99830000
H	39.44179000	17.83616000	-10.03413000
H	40.95006000	14.39952000	-8.19920000
H	41.85812000	15.71593000	-14.76689000
H	55.77537000	16.19039000	-11.21327000
H	40.41244000	12.04744000	-13.38685000
H	38.50898000	11.87850000	-5.90618000
H	26.67434436	10.29960252	-12.48912320
H	26.59508569	7.01019561	-10.29793965
H	42.90522000	8.69692000	-13.02307000
H	54.72358000	12.78633000	-7.61419000
H	54.85344000	8.99914000	-6.52715000
H	38.44640000	18.98363000	-9.12116000
H	41.43976000	15.66355000	-7.05753000
H	26.53250852	14.11532591	-13.51290973
H	42.84264000	15.80206000	-16.23804000
H	54.79085000	16.10427000	-9.74212000
H	39.91186000	12.01700000	-15.08670000
H	37.74060000	10.55130000	-6.77548000
H	27.83635095	10.66460231	-13.74195299
H	27.35717930	8.32720772	-9.43901062
H	43.68717000	8.48516000	-11.45742000
H	53.53751000	13.96012000	-7.04587000
H	54.07149000	9.21090000	-8.09280000
H	37.67802000	17.65643000	-9.99045000
H	42.62584000	14.48975000	-7.62585000
H	27.29459772	15.43233957	-12.65397915
H	43.62459000	15.59029000	-14.67239000
H	54.00891000	16.31603000	-11.30777000
H	38.73935000	11.65184000	-13.82202000
H	27.86334345	3.38004880	-6.13480928
H	53.67324453	3.41476204	-6.55955140
H	28.63990583	5.00424788	-12.01778811
H	28.64701130	10.91694189	-9.55144239
H	52.42007000	8.93694000	-4.21588000
H	52.72654033	10.95641532	-9.98697966
H	37.24861898	15.52269839	-10.11507467
H	44.16624086	19.23079932	-10.32275473
H	44.08474402	14.28167400	-12.99042682
H	37.11036866	16.78332753	-15.59178531
H	36.31044789	22.16884321	-13.13524127
H	44.02333160	21.38613601	-16.20582470
H	29.50627000	4.79996000	-8.19132000
H	51.99515000	5.87316000	-6.25728000
H	29.75636000	7.68270000	-11.28460000
H	29.44369000	11.90509000	-11.40629000
H	51.68248000	10.09555000	-6.37897000
H	51.93257000	12.97829000	-9.47225000
H	35.60358000	14.10255000	-8.05713000
H	44.48086000	18.35433000	-8.29275000
H	45.76350000	11.82290000	-13.29294000
H	36.82365000	14.67625000	-16.27229000
H	35.54100000	21.20768000	-11.27210000
H	45.70092000	18.92803000	-16.50791000
H	36.23800000	13.27392000	-6.66024000
H	28.84587000	9.16853000	-11.22369000
H	28.87186000	5.62859000	-9.58821000
H	45.15053000	10.21749000	-13.58845000
H	52.57153000	11.04375000	-7.54125000
H	52.60812000	7.47857000	-5.96176000
H	36.17541000	20.37905000	-9.87522000
H	43.59181000	17.40613000	-7.13047000
H	28.80928000	12.73372000	-12.80318000
H	45.08794000	17.32263000	-16.80343000
H	52.54554000	14.58370000	-9.17673000
H	37.73413000	13.19042000	-16.33321000
N	26.07019000	5.80794000	-6.32088000

N	55.42843000	5.18373000	-8.27186000
N	26.00761000	12.91307000	-9.53585000
N	54.20622000	11.57131000	-3.59075000
N	27.22982000	6.52549000	-14.21696000
N	55.36585000	12.28886000	-11.48683000
N	42.33022000	12.51233000	-11.27835000
N	39.03967000	13.09456000	-9.92757000
N	41.95713000	16.87857000	-11.08097000
N	39.35019000	15.83346000	-13.33993000
N	42.26764000	19.61747000	-14.49333000
N	38.97709000	20.19969000	-13.14254000
N	25.68317000	6.67245000	-7.30136000
N	54.73223000	12.50748000	-4.43063000
N	26.68464000	7.76653000	-14.36224000
N	41.96238000	11.19964000	-11.27368000
N	39.42669000	12.23005000	-8.94709000
N	55.79628000	6.49642000	-8.27654000
N	25.62059000	13.77758000	-10.51633000
N	41.89980000	18.30477000	-14.48865000
N	39.36411000	19.33518000	-12.16207000
N	55.73369000	13.60155000	-11.49151000
N	41.43112000	15.94240000	-10.24109000
N	39.89537000	14.59243000	-13.19466000
H	24.81050579	7.15918142	-7.34072631
H	25.91753836	8.00199033	-14.95899246
H	24.74792579	14.26431142	-10.55569631
H	55.97581805	4.42147889	-8.61731559
H	54.51128930	11.38591325	-2.65664039
H	55.91324144	11.52661063	-11.83228406
H	40.29935466	11.74331964	-8.90772065
H	41.09720367	10.83607026	-10.92830055
H	39.51555172	20.45129757	-13.94674930
H	25.55743037	15.24967214	-12.60983282
H	28.46579713	11.99343469	-8.18711422
H	27.23421833	10.80225626	-8.52971351
H	26.18806453	10.27035126	-14.16714077
H	53.91158571	3.07139275	-8.25612374
H	52.46603769	3.89793881	-7.72670971
H	52.96460153	10.61318426	-11.68361928
H	54.17198607	10.12988403	-10.51669591
H	43.84761403	14.62444602	-11.29356401
H	45.29272129	13.79796768	-11.82428541
H	44.51238790	18.19231122	-11.68466198
H	43.08347227	19.19788788	-11.69373821
H	43.78405574	21.72996495	-14.50947704
H	45.22994908	20.90337835	-15.03788379
H	36.77327996	17.11778737	-13.91024599
H	38.18641258	17.80761933	-14.67199052
H	37.49112900	14.47741833	-11.49407617
H	36.05507081	14.31014268	-10.51284103
H	36.55087822	21.12247297	-14.51378007
H	37.74575267	22.33433323	-14.11788054
H	28.97699453	4.66978804	-13.69932743
H	30.05303844	5.69407985	-12.77953264
H	25.62001161	8.14454429	-9.39486142
H	27.61698626	4.42330638	-4.75495841
H	29.05443151	4.59388542	-5.73359043
H	41.72024896	20.37972164	-14.14788032