

113

IS, "bridge"-diffusion ENERGY(Rydberg)= -5934.93724979

Pt	0.0000000000	0.0000000000	-13.7190560799
Pt	-1.4001952976	2.4252093963	-13.7190560799
Pt	2.8003905958	0.0000000000	-13.7190560799
Pt	1.4001952976	2.4252093963	-13.7190560799
Pt	0.0000000000	1.6168062642	-11.4325467335
Pt	-1.4001952976	4.0420156606	-11.4325467335
Pt	2.8003905958	1.6168062642	-11.4325467335
Pt	1.4001952976	4.0420156606	-11.4325467335
Pt	1.3999894611	0.8107467837	-9.1606550701
Pt	-0.0000963727	3.2348872744	-9.1542992650
Pt	4.2026887096	0.8101371653	-9.1582975863
Pt	2.8002058751	3.2348476394	-9.1542737659
Pt	0.0004228058	-0.0001741466	-6.8922205438
Pt	-1.3998288180	2.4271996087	-6.8777256452
Pt	2.8007565463	0.0002512168	-6.8917300674
Pt	1.4004529051	2.4282912331	-6.8772308634
Pt	-0.0016493121	1.6183896157	-4.6095620243
Pt	-1.3951469992	4.0451694426	-4.5911697772
Pt	2.8014405524	1.6183797440	-4.6087753407
Pt	1.3996312467	4.0420839629	-4.5872248474
Pt	1.3976878443	0.8103888460	-2.3468875345
Pt	-0.0074358063	3.2415908146	-2.3062495341
Pt	4.1956569961	0.8079141044	-2.3344397417
Pt	2.8037985946	3.2413675059	-2.3068337567
Pt	-0.0031100213	0.0019581981	-0.0200447341
Pt	-1.4172015648	2.4135259595	-0.0131593451
Pt	2.7952139403	0.0015015469	-0.0187389076
Pt	1.3967057204	2.3911784316	-0.0294962268
Pt	-2.8004007099	4.8504363116	-13.7190560799
Pt	5.6008014199	0.0000000000	-13.7190560799
Pt	2.8004007099	4.8504363116	-13.7190560799
Pt	-4.2005960076	7.2756457079	-13.7190560799
Pt	4.2006061223	2.4252093963	-13.7190560799
Pt	1.4002054123	7.2756457079	-13.7190560799
Pt	-0.0000101142	4.8504363116	-13.7190560799
Pt	8.4011920156	0.0000000000	-13.7190560799
Pt	5.6007913057	4.8504363116	-13.7190560799
Pt	-1.4002054123	7.2756457079	-13.7190560799
Pt	7.0009967175	2.4252093963	-13.7190560799
Pt	4.2005960076	7.2756457079	-13.7190560799
Pt	-2.8004007099	6.4672425758	-11.4325467335
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Pt	-4.2005960076	8.8924519722	-11.4325467335
Pt	4.2006061223	4.0420156606	-11.4325467335
Pt	1.4002054123	8.8924519722	-11.4325467335
Pt	-0.0000101142	6.4672425758	-11.4325467335
Pt	8.4011920156	1.6168062642	-11.4325467335
Pt	5.6007913057	6.4672425758	-11.4325467335
Pt	-1.4002054123	8.8924519722	-11.4325467335
Pt	7.0009967175	4.0420156606	-11.4325467335
Pt	4.2005960076	8.8924519722	-11.4325467335
Pt	-1.3994025302	5.6587034902	-9.1541327790
Pt	7.0008552332	0.8071056020	-9.1564185845
Pt	4.1994500218	5.6584364730	-9.1544924376
Pt	-2.7991672434	8.0833637541	-9.1608968869
Pt	5.5999276666	3.2340654375	-9.1558709743
Pt	2.7993162531	8.0836442065	-9.1543325018
Pt	1.4001546127	5.6588832395	-9.1522817393
Pt	9.7989294586	0.8098797516	-9.1578775220
Pt	7.0005595157	5.6561900676	-9.1583252554

Pt	0.0005460450	8.0834242208	-9.1541714993
Pt	8.4021456435	3.2344564216	-9.1564750996
Pt	5.5987953785	8.0832638785	-9.1607235322
Pt	-2.7986797846	4.8493162326	-6.8775623815
Pt	5.6027222666	-0.0009083800	-6.8776541771
Pt	2.7997054393	4.8509038607	-6.8703795083
Pt	-4.2005763333	7.2753960228	-6.8917626659
Pt	4.2008497544	2.4269645177	-6.8767191243
Pt	1.4005623104	7.2741988044	-6.8702618285
Pt	0.0013735317	4.8509778082	-6.8702591962
Pt	8.3998170163	-0.0011865122	-6.8776163625
Pt	5.5994729646	4.8493512820	-6.8769881654
Pt	-1.3970844066	7.2739775962	-6.8776396182
Pt	7.0014221905	2.4250721856	-6.8847544388
Pt	4.1982424975	7.2740861827	-6.8773505453
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Pt	5.6023114735	1.6181865265	-4.6083706114
Pt	2.8002569870	6.4678947548	-4.5878078841
Pt	-4.2003314099	8.8925679357	-4.6186688786
Pt	4.1948068082	4.0452913883	-4.5914467762
Pt	1.4001202747	8.8866509130	-4.5914297518
Pt	-0.0003970501	6.4675446131	-4.5865671204
Pt	8.3991825748	1.6180813228	-4.6091914738
Pt	5.6000821507	6.4657640670	-4.6092780966
Pt	-1.3981041269	8.8929370819	-4.6097288189
Pt	7.0007640023	4.0402038603	-4.6081878930
Pt	4.1986081022	8.8931644445	-4.6097252409
Pt	-1.3986713163	5.6528547177	-2.3051172719
Pt	6.9985735752	0.8168254449	-2.3314484643
Pt	4.1956605234	5.6522086461	-2.3068952578
Pt	-2.8023741340	8.0851936006	-2.3465652736
Pt	5.6047843345	3.2314540471	-2.3302401170
Pt	2.7898030432	8.0862837016	-2.3063102050
Pt	1.3985554972	5.6599254920	-2.2902350842
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Pt	6.9990842881	5.6635302880	-2.3344351769
Pt	0.0058877209	8.0859852576	-2.3057814476
Pt	8.3928684523	3.2316376739	-2.3313633472
Pt	5.5981080118	8.0854684664	-2.3466331846
Pt	-2.8227568209	4.8481139800	-0.0126458659
Pt	5.5915876187	0.0208541375	-0.0131824404
Pt	2.8559092775	4.8185927608	0.0676554244
Pt	-4.2046070849	7.2795662155	-0.0192830616
Pt	4.2112536132	2.4116074992	-0.0125311254
Pt	1.3959628309	7.3457208628	0.0723515298
Pt	-0.0623348494	4.8193853883	0.0727752437
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Pt	5.6181534006	4.8483513751	-0.0127988223
Pt	-1.4359369454	7.2964715547	-0.0287577448
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TS, "bridge"-diffusion ENERGY(Rydberg)= -5934.86675154

Pt	0.0000000000	0.0000000000	-13.7190560799
Pt	-1.4001952976	2.4252093963	-13.7190560799
Pt	2.8003905958	0.0000000000	-13.7190560799
Pt	1.4001952976	2.4252093963	-13.7190560799
Pt	0.0000000000	1.6168062642	-11.4325467335
Pt	-1.4001952976	4.0420156606	-11.4325467335
Pt	2.8003905958	1.6168062642	-11.4325467335
Pt	1.4001952976	4.0420156606	-11.4325467335
Pt	1.4007900626	0.8085587238	-9.1571337476

Pt	0.0006421142	3.2343501849	-9.1574506386
Pt	4.2004967299	0.8086599369	-9.1565374234
Pt	2.7999867759	3.2340032990	-9.1569670641
Pt	0.0006941396	0.0001562899	-6.8847463242
Pt	-1.4009277244	2.4261743578	-6.8838955269
Pt	2.8020633736	-0.0001982336	-6.8790242674
Pt	1.4003667888	2.4257168141	-6.8795467158
Pt	-0.0001742932	1.6199206747	-4.6100988475
Pt	-1.3989150581	4.0397633922	-4.6089006693
Pt	2.8011396695	1.6264588060	-4.6064072787
Pt	1.4057715386	4.0455624729	-4.5926112731
Pt	1.3988548224	0.8105348494	-2.3354501064
Pt	0.0010715723	3.2386426212	-2.3310416994
Pt	4.1953649705	0.8088454027	-2.2999081517
Pt	2.8051927928	3.2372393274	-2.2827655831
Pt	-0.0058727454	0.0032057767	-0.0149367629
Pt	-1.4045578079	2.4281013969	-0.0162523262
Pt	2.7939502918	-0.0039971322	0.0022140160
Pt	1.3856495244	2.3977058142	-0.0191148168
Pt	-2.8004007099	4.8504363116	-13.7190560799
Pt	5.6008014199	0.0000000000	-13.7190560799
Pt	2.8004007099	4.8504363116	-13.7190560799
Pt	-4.2005960076	7.2756457079	-13.7190560799
Pt	4.2006061223	2.4252093963	-13.7190560799
Pt	1.4002054123	7.2756457079	-13.7190560799
Pt	-0.0000101142	4.8504363116	-13.7190560799
Pt	8.4011920156	0.0000000000	-13.7190560799
Pt	5.6007913057	4.8504363116	-13.7190560799
Pt	-1.4002054123	7.2756457079	-13.7190560799
Pt	7.0009967175	2.4252093963	-13.7190560799
Pt	4.2005960076	7.2756457079	-13.7190560799
Pt	-2.8004007099	6.4672425758	-11.4325467335
Pt	5.6008014199	1.6168062642	-11.4325467335
Pt	2.8004007099	6.4672425758	-11.4325467335
Pt	-4.2005960076	8.8924519722	-11.4325467335
Pt	4.2006061223	4.0420156606	-11.4325467335
Pt	1.4002054123	8.8924519722	-11.4325467335
Pt	-0.0000101142	6.4672425758	-11.4325467335
Pt	8.4011920156	1.6168062642	-11.4325467335
Pt	5.6007913057	6.4672425758	-11.4325467335
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Pt	7.0009967175	4.0420156606	-11.4325467335
Pt	4.2005960076	8.8924519722	-11.4325467335
Pt	-1.4000315353	5.6593875536	-9.1601817786
Pt	7.0000656049	0.8083489270	-9.1576902345
Pt	4.2003570328	5.6591187977	-9.1574863972
Pt	-2.7989530794	8.0848929784	-9.1572360612
Pt	5.5999367802	3.2341841782	-9.1578385785
Pt	2.8000286847	8.0832349807	-9.1569712785
Pt	1.4005211416	5.6595017971	-9.1560198423
Pt	9.8010908581	0.8082463576	-9.1590692063
Pt	7.0007294671	5.6583548244	-9.1564919301
Pt	0.0002363960	8.0847744081	-9.1561198620
Pt	8.4010778028	3.2343861036	-9.1580255138
Pt	5.6006581223	8.0834155516	-9.1587686515
Pt	-2.8000857389	4.8525523684	-6.8795310581
Pt	5.6001162791	-0.0014914291	-6.8770069758
Pt	2.8004159134	4.8513025045	-6.8783142299
Pt	-4.1970376763	7.2772701931	-6.8853628487
Pt	4.2000068578	2.4248578253	-6.8794181349
Pt	1.4016047368	7.2747487416	-6.8775721183
Pt	-0.0005777647	4.8510037091	-6.8796365733
Pt	8.4010388059	-0.0005673631	-6.8843291133

Pt	5.6001945319	4.8509458742	-6.8793766257
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Pt	7.0013157489	2.4243022260	-6.8845461406
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Pt	-2.8007384354	6.4687421771	-4.5990613003
Pt	5.5968315535	1.6172302106	-4.5989690512
Pt	2.8068509158	6.4622015224	-4.5919554105
Pt	-4.2011217157	8.8955130248	-4.6089479545
Pt	4.1988388716	4.0431680301	-4.6026393136
Pt	1.4024518040	8.8927706187	-4.6074470753
Pt	0.0080250219	6.4644327586	-4.6064139531
Pt	8.3982134310	1.6173972901	-4.6088139644
Pt	5.6018889288	6.4640241038	-4.6100784399
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Pt	6.9997902932	4.0385739403	-4.6094122424
Pt	4.1987967781	8.8937161966	-4.6120868364
Pt	-1.3994632800	5.6652181934	-2.3376943675
Pt	6.9953823895	0.8105561125	-2.3276958728
Pt	4.1972589648	5.6501045289	-2.2868541321
Pt	-2.8034600183	8.0895093064	-2.3268676521
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Pt	2.7944417845	8.0847039331	-2.3346477372
Pt	1.4158608033	5.6531058863	-2.2982658632
Pt	9.7975106124	0.8109208731	-2.3355537094
Pt	7.0014402261	5.6650059977	-2.3389551794
Pt	-0.0064035862	8.0859365838	-2.3349008921
Pt	8.3991749408	3.2381133727	-2.3323231761
Pt	5.6012913778	8.0859815535	-2.3439506508
Pt	-2.8018581073	4.8539652052	-0.0108914281
Pt	5.6061929058	0.0010846181	0.0053717530
Pt	2.8118362848	4.8737142034	0.0971447790
Pt	-4.1963778245	7.2851381586	-0.0131378385
Pt	4.2219298810	2.3965635223	-0.0054801121
Pt	1.3766273913	7.3120942655	-0.0303674939
Pt	-0.0379710259	4.8605302331	-0.0316243294
Pt	8.4006450747	0.0122079814	-0.0138275788
Pt	5.6434329164	4.8554460227	-0.0262564375
Pt	-1.4098181550	7.2857831858	-0.0081642353
Pt	7.0076247460	2.4256305229	-0.0069598680
Pt	4.2181550666	7.3133295029	-0.0384916688
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FS, "bridge"-diffusion ENERGY(Rydberg)= -5934.96829753

Pt	0.0000000000	0.0000000000	-13.7190560799
Pt	-1.4001952976	2.4252093963	-13.7190560799
Pt	2.8003905958	0.0000000000	-13.7190560799
Pt	1.4001952976	2.4252093963	-13.7190560799
Pt	0.0000000000	1.6168062642	-11.4325467335
Pt	-1.4001952976	4.0420156606	-11.4325467335
Pt	2.8003905958	1.6168062642	-11.4325467335
Pt	1.4001952976	4.0420156606	-11.4325467335
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Pt	4.2004967299	0.8086582490	-9.1565374234
Pt	2.8006048910	3.2340032990	-9.1575266021
Pt	0.0005109049	-0.0004123028	-6.8847463242
Pt	-1.4001649106	2.4261743578	-6.8849816081
Pt	2.8020633736	-0.0011294525	-6.8790242674
Pt	1.3996267226	2.4257168141	-6.8823816642
Pt	-0.0001742932	1.6175328437	-4.6100988475
Pt	-1.4014798453	4.0397633922	-4.6086695039
Pt	2.8011396695	1.6160636647	-4.6064072787
Pt	1.3978545249	4.0455624729	-4.6059544783

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Pt	4.1979249640	0.8313532808	-2.2999081517
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Pt	-1.4029152350	2.4226221947	-0.0134644644
Pt	2.7823998164	-0.0258064449	-0.0098191680
Pt	1.3657553624	2.4103781490	-0.0379051151
Pt	-2.8004007099	4.8504363116	-13.7190560799
Pt	5.6008014199	0.0000000000	-13.7190560799
Pt	2.8004007099	4.8504363116	-13.7190560799
Pt	-4.2005960076	7.2756457079	-13.7190560799
Pt	4.2006061223	2.4252093963	-13.7190560799
Pt	1.4002054123	7.2756457079	-13.7190560799
Pt	-0.0000101142	4.8504363116	-13.7190560799
Pt	8.4011920156	0.0000000000	-13.7190560799
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Pt	-1.4002054123	7.2756457079	-13.7190560799
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Pt	4.2005960076	7.2756457079	-13.7190560799
Pt	-2.8004007099	6.4672425758	-11.4325467335
Pt	5.6008014199	1.6168062642	-11.4325467335
Pt	2.8004007099	6.4672425758	-11.4325467335
Pt	-4.2005960076	8.8924519722	-11.4325467335
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Pt	4.2005960076	8.8924519722	-11.4325467335
Pt	-1.4000315353	5.6571767767	-9.1601817786
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Pt	4.2003570328	5.6584404523	-9.1574863972
Pt	-2.8020326145	8.0848929784	-9.1603986949
Pt	5.5999367802	3.2340415039	-9.1578385785
Pt	2.8003720009	8.0832349807	-9.1574012698
Pt	1.4005211416	5.6586449394	-9.1560198423
Pt	9.8016920593	0.8082463576	-9.1590049637
Pt	7.0007294671	5.6587284814	-9.1564919301
Pt	0.0014921400	8.0847744081	-9.1602981625
Pt	8.4010778028	3.2339377442	-9.1575249293
Pt	5.6009419052	8.0834155516	-9.1573658935
Pt	-2.8000857389	4.8529937053	-6.8795310581
Pt	5.5986809228	-0.0014914291	-6.8796032724
Pt	2.8004159134	4.8504032012	-6.8783142299
Pt	-4.1987151049	7.2746110892	-6.8790332923
Pt	4.2000068578	2.4255162511	-6.8794181349
Pt	1.3975457792	7.2747487416	-6.8791388738
Pt	-0.0005777647	4.8531501276	-6.8789190771
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Pt	4.1999410860	7.2759035805	-6.8824144461
Pt	-2.8007384354	6.4682456586	-4.5990613003
Pt	5.5971596515	1.6163567023	-4.6084292965
Pt	2.7960872286	6.4675457195	-4.6061398055
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Pt	4.1988388716	4.0431680301	-4.6026393136
Pt	1.4014433744	8.8947633500	-4.6089697854
Pt	-0.0021755586	6.4686614157	-4.5982792735

Pt	8.3986569407	1.6183142110	-4.6114013422
Pt	5.6018889288	6.4671158633	-4.6065926116
Pt	-1.4012854876	8.8924606805	-4.5991288908
Pt	6.9997193272	4.0456090278	-4.6085034727
Pt	4.1995695835	8.8922904847	-4.6099412071
Pt	-1.4031772608	5.6644128064	-2.3311256936
Pt	6.9951305368	0.8088527062	-2.3373012803
Pt	4.1972589648	5.6582239884	-2.3251066866
Pt	-2.8001784930	8.0842989393	-2.3324519422
Pt	5.5958791644	3.2370003780	-2.3268479485
Pt	2.7944417845	8.0847039331	-2.3360754687
Pt	1.4143967257	5.6508396856	-2.2982658632
Pt	9.7975106124	0.8109208731	-2.3336207075
Pt	6.9800628515	5.6503308857	-2.3000670664
Pt	-0.0060301875	8.0843312596	-2.3309802273
Pt	8.3980982877	3.2389111199	-2.3372169653
Pt	5.6000992362	8.0851811335	-2.3363112005
Pt	-2.7717998223	4.8543692316	-0.0090992286
Pt	5.6125084041	-0.0259129409	-0.0090689654
Pt	2.7096164692	4.9034301158	0.0104406369
Pt	-4.1869047213	7.3051205561	-0.0102116459
Pt	4.1986710454	2.3269746020	0.0072261606
Pt	1.3794792854	7.3051108411	-0.0078269568
Pt	-0.0353852142	4.8544698815	-0.0077014686
Pt	8.4027989002	0.0047523057	-0.0136748155
Pt	5.6854401377	4.9021758174	0.0074920914
Pt	-1.4043148964	7.2786523592	0.0056217145
Pt	7.0307739698	2.4086803533	-0.0394251029
Pt	4.1968908839	7.3137306815	-0.0384916688
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