

Electronic Energy (BLYP/6-31G*)	-570.04949
Sum of electronic and zero-point Energies	-569.91382
Sum of electronic and thermal Energies	-569.90242
Sum of electronic and thermal Enthalpies	-569.90147
Sum of electr. and thermal Free Energies	-569.95092
Electronic Energy (BLYP/6-311+G**)	-570.20798
38. [4,5]Benzo-3,6-Diazacyclodeca-3,7,9-triene-1,5-diyne (11mr)	
Electronic Energy (BLYP/6-31G*)	-570.04673
Sum of electronic and zero-point Energies	-569.90847
Sum of electronic and thermal Energies	-569.89798
Sum of electronic and thermal Enthalpies	-569.89703
Sum of electr. and thermal Free Energies	-569.94432
Electronic Energy (BLYP/6-311+G**)	-570.19824
(6.1)	
39. 1,2-Diethynyl-1,4-cyclohexadiene (48e)	
Electronic Energy (BLYP/6-31G*)	-385.53526
Sum of electronic and zero-point Energies	-385.39991
Sum of electronic and thermal Energies	-385.38999
Sum of electronic and thermal Enthalpies	-385.38905
Sum of electr. and thermal Free Energies	-385.43471
Electronic Energy (BLYP/6-311+G**)	-385.65212
40. 2,3-Diethynylpyrrole (49e)	
Electronic Energy (BLYP/6-31G*)	-362.32614
Sum of electronic and zero-point Energies	-362.22936
Sum of electronic and thermal Energies	-362.22083
Sum of electronic and thermal Enthalpies	-362.21989
Sum of electr. and thermal Free Energies	-362.26211
Electronic Energy (BLYP/6-311+G**)	-362.44022
41. 3,4-Diethynylpyrrole (50e)	
Electronic Energy (BLYP/6-31G*)	-362.32364
Sum of electronic and zero-point Energies	-362.22697
Sum of electronic and thermal Energies	-362.21841
Sum of electronic and thermal Enthalpies	-362.21747
Sum of electr. and thermal Free Energies	-362.25973
Electronic Energy (BLYP/6-311+G**)	-362.43799
42. 2H-1,2-Diaza-3,4-Diethynylcyclopentadiene (51e)	
Electronic Energy (BLYP/6-31G*)	-378.36844
Sum of electronic and zero-point Energies	-378.28280
Sum of electronic and thermal Energies	-378.27457
Sum of electronic and thermal Enthalpies	-378.27363
Sum of electr. and thermal Free Energies	-378.31540
Electronic Energy (BLYP/6-311+G**)	-378.48556
43. 4,5-Diethynylimidazole (52e)	
Electronic Energy (BLYP/6-31G*)	-378.38341

Sum of electronic and zero-point Energies	-378.29809
Sum of electronic and thermal Energies	-378.28983
Sum of electronic and thermal Enthalpies	-378.28889
Sum of electr. and thermal Free Energies	-378.33069
Electronic Energy (BLYP/6-311+G**)	-378.50152

44. 4,5-Diethynylimidazolium Ion (53e)	
Electronic Energy (BLYP/6-31G*)	-378.75797
Sum of electronic and zero-point Energies	-378.65840
Sum of electronic and thermal Energies	-378.65035
Sum of electronic and thermal Enthalpies	-378.64941
Sum of electr. and thermal Free Energies	-378.69090
Electronic Energy (BLYP/6-311+G**)	-378.86757

45. 1,2-Diethynylcyclobutane (54e)	
Electronic Energy (BLYP/6-31G*)	-308.14180
Sum of electronic and zero-point Energies	-308.04016
Sum of electronic and thermal Energies	-308.03206
Sum of electronic and thermal Enthalpies	-308.03112
Sum of electr. and thermal Free Energies	-308.07238
Electronic Energy (BLYP/6-311+G**)	-308.23587

46a. Cyclooct-3-ene-1,5-diyne, planar (54mr)	
Electronic Energy (BLYP/6-31G*)	-308.14968
Sum of electronic and zero-point Energies	-308.04477
Sum of electronic and thermal Energies	-308.03824
Sum of electronic and thermal Enthalpies	-308.03730
Sum of electr. and thermal Free Energies	-308.07503
Electronic Energy (BLYP/6-311+G**)	-308.24216

46b. Cyclooct-3-ene-1,5-diyne, non-planar (54mr')	
Electronic Energy (BLYP/6-31G*)	-308.14969
Sum of electronic and zero-point Energies	-308.04466
Sum of electronic and thermal Energies	-308.03729
Sum of electronic and thermal Enthalpies	-308.03634
Sum of electr. and thermal Free Energies	-308.07650
Electronic Energy (BLYP/6-311+G**)	-308.24216

II. TRANSITION STATES (44 structures).

1. 1e to 1p (1t)	
Electronic Energy (BLYP/6-31G*)	-230.74785
Sum of electronic and zero-point Energies	-230.67994
Sum of electronic and thermal Energies	-230.67480
Sum of electronic and thermal Enthalpies	-230.67385
Sum of electr. and thermal Free Energies	-230.70782
Electronic Energy (BLYP/6-311+G**)	-230.81967
Electronic Energy (BLYP/cc-pVTZ)	-230.83949
Electronic Energy (BPW91/6-31G*)	-230.81184

2. 26e to 26p (26t)			
Electronic Energy (BLYP/6-31G*)	-270.03938	Sum of electronic and thermal Energies	-429.13462
Sum of electronic and zero-point Energies	-269.94420	Sum of electronic and thermal Enthalpies	-429.13368
Sum of electronic and thermal Energies	-269.93742	Sum of electr. and thermal Free Energies	-429.17233
Sum of electronic and thermal Enthalpies	-269.93648	Electronic Energy (BLYP/6-311+G**)	-429.33902
Sum of electr. and thermal Free Energies	-269.97429		
Electronic Energy (BLYP/6-311+G**)	-270.12182		
3. 27e to 27p (27t)			
Electronic Energy (BLYP/6-31G*)	-344.05436		
Sum of electronic and zero-point Energies	-343.97730		
Sum of electronic and thermal Energies	-343.97030		
Sum of electronic and thermal Enthalpies	-343.96935		
Sum of electr. and thermal Free Energies	-344.00836		
Electronic Energy (BLYP/6-311+G**)	-344.16095		
4. 21e to 21p (21t)			
Electronic Energy (BLYP/6-31G*)	-690.32774		
Sum of electronic and zero-point Energies	-690.26923		
Sum of electronic and thermal Energies	-690.26288		
Sum of electronic and thermal Enthalpies	-690.26194		
Sum of electr. and thermal Free Energies	-690.29961		
Electronic Energy (BLYP/6-311+G**)	-690.42738		
5. 25e to 21p (25t)			
Electronic Energy (BLYP/6-31G*)	-690.32513		
Sum of electronic and zero-point Energies	-690.26575		
Sum of electronic and thermal Energies	-690.25947		
Sum of electronic and thermal Enthalpies	-690.25852		
Sum of electr. and thermal Free Energies	-690.29630		
Electronic Energy (BLYP/6-311+G**)	-690.42362		
6. 22e to 22p (22t)			
Electronic Energy (BLYP/6-31G*)	-1149.90201		
Sum of electronic and zero-point Energies	-1149.85295		
Sum of electronic and thermal Energies	-1149.84529		
Sum of electronic and thermal Enthalpies	-1149.84434		
Sum of electr. and thermal Free Energies	-1149.88581		
Electronic Energy (BLYP/6-311+G**)	-1150.02964		
7. 19e to 19p (19t)			
Electronic Energy (BLYP/6-31G*)	-329.97533		
Sum of electronic and zero-point Energies	-329.91557		
Sum of electronic and thermal Energies	-329.90950		
Sum of electronic and thermal Enthalpies	-329.90855		
Sum of electr. and thermal Free Energies	-329.94506		
Electronic Energy (BLYP/6-311+G**)	-330.08396		
8. 20e to 20p (20t)			
Electronic Energy (BLYP/6-31G*)	-429.19355		
Sum of electronic and zero-point Energies	-429.14151		
		Sum of electronic and thermal Energies	-429.13462
		Sum of electronic and thermal Enthalpies	-429.13368
		Sum of electr. and thermal Free Energies	-429.17233
		Electronic Energy (BLYP/6-311+G**)	-429.33902
		9. 28e to 28p (28t)	
		Electronic Energy (BLYP/6-31G*)	-435.24077
		Sum of electronic and zero-point Energies	-435.17091
		Sum of electronic and thermal Energies	-435.16330
		Sum of electronic and thermal Enthalpies	-435.16236
		Sum of electr. and thermal Free Energies	-435.20337
		Electronic Energy (BLYP/6-311+G**)	-435.37676
		10. 29e to 29p (29t)	
		Electronic Energy (BLYP/6-31G*)	-305.95696
		Sum of electronic and zero-point Energies	-305.88563
		Sum of electronic and thermal Energies	-305.87896
		Sum of electronic and thermal Enthalpies	-305.87802
		Sum of electr. and thermal Free Energies	-305.91578
		Electronic Energy (BLYP/6-311+G**)	-306.06142
		11. 30e to 30p (30t)	
		Electronic Energy (BLYP/6-31G*)	-419.27451
		Sum of electronic and zero-point Energies	-419.19389
		Sum of electronic and thermal Energies	-419.18557
		Sum of electronic and thermal Enthalpies	-419.18463
		Sum of electr. and thermal Free Energies	-419.22698
		Electronic Energy (BLYP/6-311+G**)	-419.40594
		12. 31e to 31p (31t)	
		Electronic Energy (BLYP/6-31G*)	-286.08516
		Sum of electronic and zero-point Energies	-286.00112
		Sum of electronic and thermal Energies	-285.99444
		Sum of electronic and thermal Enthalpies	-285.99349
		Sum of electr. and thermal Free Energies	-286.03087
		Electronic Energy (BLYP/6-311+G**)	-286.18165
		13. 31e' to 31p (31t')	
		Electronic Energy (BLYP/6-31G*)	-286.08399
		Sum of electronic and zero-point Energies	-285.99934
		Sum of electronic and thermal Energies	-285.99274
		Sum of electronic and thermal Enthalpies	-285.99180
		Sum of electr. and thermal Free Energies	-286.02923
		Electronic Energy (BLYP/6-311+G**)	-286.17874
		14. 32e to 32p (32t)	
		Electronic Energy (BLYP/6-31G*)	-286.08253
		Sum of electronic and zero-point Energies	-286.00004
		Sum of electronic and thermal Energies	-285.99402
		Sum of electronic and thermal Enthalpies	-285.99307
		Sum of electr. and thermal Free Energies	-286.02936

Electronic Energy (BLYP/6-311+G**) -286.17970

15. 33e to 33p (33t)

Electronic Energy (BLYP/6-31G*) -286.06344
Sum of electronic and zero-point Energies -285.98127
Sum of electronic and thermal Energies -285.97528
Sum of electronic and thermal Enthalpies -285.97433
Sum of electr. and thermal Free Energies -286.01065
Electronic Energy (BLYP/6-311+G**) -286.16199

16. 34e to 34p (34t)

Electronic Energy (BLYP/6-31G*) -399.41004
Sum of electronic and zero-point Energies -399.31660
Sum of electronic and thermal Energies -399.30814
Sum of electronic and thermal Enthalpies -399.30720
Sum of electr. and thermal Free Energies -399.34963
Electronic Energy (BLYP/6-311+G**) -399.53810

17. 39e to 39p (39t)

Electronic Energy (BLYP/6-31G*) -628.91661
Sum of electronic and zero-point Energies -628.85002
Sum of electronic and thermal Energies -628.84284
Sum of electronic and thermal Enthalpies -628.84190
Sum of electr. and thermal Free Energies -628.88123
Electronic Energy (BLYP/6-311+G**) -629.01922

18. 40e to 40p (40t)

Electronic Energy (BLYP/6-31G*) -704.07189
Sum of electronic and zero-point Energies -704.00099
Sum of electronic and thermal Energies -703.99316
Sum of electronic and thermal Enthalpies -703.99222
Sum of electr. and thermal Free Energies -704.03398
Electronic Energy (BLYP/6-311+G**) -704.20170

19. 36e to 36p (36t)

Electronic Energy (BLYP/6-31G*) -256.17357
Sum of electronic and zero-point Energies -256.09422
Sum of electronic and thermal Energies -256.08764
Sum of electronic and thermal Enthalpies -256.08670
Sum of electr. and thermal Free Energies -256.12398
Electronic Energy (BLYP/6-311+G**) -256.24767

20. 37e to 37p (37t)

Electronic Energy (BLYP/6-31G*) -256.15821
Sum of electronic and zero-point Energies -256.08061
Sum of electronic and thermal Energies -256.07410
Sum of electronic and thermal Enthalpies -256.07316
Sum of electr. and thermal Free Energies -256.11045
Electronic Energy (BLYP/6-311+G**) -256.23346

21. 35e to 35p (35t)

Electronic Energy (BLYP/6-31G*) -286.47136
Sum of electronic and zero-point Energies -286.37274
Sum of electronic and thermal Energies -286.36468
Sum of electronic and thermal Enthalpies -286.36373
Sum of electr. and thermal Free Energies -286.40478
Electronic Energy (BLYP/6-311+G**) -286.56273

22. 38e to 38p (38t)

Electronic Energy (BLYP/6-31G*) -256.80792
Sum of electronic and zero-point Energies -256.72259
Sum of electronic and thermal Energies -256.71526
Sum of electronic and thermal Enthalpies -256.71432
Sum of electr. and thermal Free Energies -256.75318
Electronic Energy (BLYP/6-311+G**) -256.90279

23. 23e to 23p (23t)

Electronic Energy (BLYP/6-31G*) -347.42011
Sum of electronic and zero-point Energies -347.28931
Sum of electronic and thermal Energies -347.28160
Sum of electronic and thermal Enthalpies -347.28066
Sum of electr. and thermal Free Energies -347.32105
Electronic Energy (BLYP/6-311+G**) -347.52067

24. 41e to 41p (41t)

Electronic Energy (BLYP/6-31G*) -461.70226
Sum of electronic and zero-point Energies -461.55568
Sum of electronic and thermal Energies -461.54583
Sum of electronic and thermal Enthalpies -461.54489
Sum of electr. and thermal Free Energies -461.59131
Electronic Energy (BLYP/6-311+G**) -461.83187

25. 42e to 42p (42t)

Electronic Energy (BLYP/6-31G*) -560.93575
Sum of electronic and zero-point Energies -560.79732
Sum of electronic and thermal Energies -560.78658
Sum of electronic and thermal Enthalpies -560.78564
Sum of electr. and thermal Free Energies -560.83428
Electronic Energy (BLYP/6-311+G**) -561.10328

26. 43e to 43p (43t)

Electronic Energy (BLYP/6-31G*) -487.12475
Sum of electronic and zero-point Energies -486.96706
Sum of electronic and thermal Energies -486.95564
Sum of electronic and thermal Enthalpies -486.95470
Sum of electr. and thermal Free Energies -487.00456
Electronic Energy (BLYP/6-311+G**) -487.25673

27. 17e to 17p (17t)

Electronic Energy (BLYP/6-31G*) -386.71491
Sum of electronic and zero-point Energies -386.55399

Sum of electronic and thermal Energies	-386.54555
Sum of electronic and thermal Enthalpies	-386.54461
Sum of electr. and thermal Free Energies	-386.58713
Electronic Energy (BLYP/6-311+G**)	-386.82384

28. 13e to 13p (13t)

Electronic Energy (BLYP/6-31G*)	-846.29523
Sum of electronic and zero-point Energies	-846.14381
Sum of electronic and thermal Energies	-846.13400
Sum of electronic and thermal Enthalpies	-846.13306
Sum of electr. and thermal Free Energies	-846.17945
Electronic Energy (BLYP/6-311+G**)	-846.43209

29. 9e to 9p (9t)

Electronic Energy (BLYP/6-31G*)	-384.33869
Sum of electronic and zero-point Energies	-384.22434
Sum of electronic and thermal Energies	-384.21682
Sum of electronic and thermal Enthalpies	-384.21588
Sum of electr. and thermal Free Energies	-384.25600
Electronic Energy (BLYP/6-311+G**)	-384.44573

30. 9mr to 9p (9ot)

Electronic Energy (BLYP/6-31G*)	-384.34459
Sum of electronic and zero-point Energies	-384.22922
Sum of electronic and thermal Energies	-384.22202
Sum of electronic and thermal Enthalpies	-384.22107
Sum of electr. and thermal Free Energies	-384.26073
Electronic Energy (BLYP/6-311+G**)	-384.44869

31. 45e to 45p (45t)

Electronic Energy (BLYP/6-31G*)	-483.57155
Sum of electronic and zero-point Energies	-483.46540
Sum of electronic and thermal Energies	-483.45700
Sum of electronic and thermal Enthalpies	-483.45606
Sum of electr. and thermal Free Energies	-483.49837
Electronic Energy (BLYP/6-311+G**)	-483.71641

32. 10e to 10p (10t)

Electronic Energy (BLYP/6-31G*)	-400.38522
Sum of electronic and zero-point Energies	-400.28284
Sum of electronic and thermal Energies	-400.27543
Sum of electronic and thermal Enthalpies	-400.27449
Sum of electr. and thermal Free Energies	-400.31450
Electronic Energy (BLYP/6-311+G**)	-400.49633

33. 46e to 46p (46t)

Electronic Energy (BLYP/6-31G*)	-416.43617
Sum of electronic and zero-point Energies	-416.34533
Sum of electronic and thermal Energies	-416.33805
Sum of electronic and thermal Enthalpies	-416.33710
Sum of electr. and thermal Free Energies	-416.37698

Electronic Energy (BLYP/6-311+G**)	-416.55113
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34. 46mr to 46p (46ot)

Electronic Energy (BLYP/6-31G*)	-416.44949
Sum of electronic and zero-point Energies	-416.35738
Sum of electronic and thermal Energies	-416.35044
Sum of electronic and thermal Enthalpies	-416.34950
Sum of electr. and thermal Free Energies	-416.38885
Electronic Energy (BLYP/6-311+G**)	-416.56076

35. 47e to 47p (47t)

Electronic Energy (BLYP/6-31G*)	-416.42907
Sum of electronic and zero-point Energies	-416.33888
Sum of electronic and thermal Energies	-416.33154
Sum of electronic and thermal Enthalpies	-416.33060
Sum of electr. and thermal Free Energies	-416.37060
Electronic Energy (BLYP/6-311+G**)	-416.54409

36. 11e to 11p (11t)

Electronic Energy (BLYP/6-31G*)	-570.01196
Sum of electronic and zero-point Energies	-569.87644
Sum of electronic and thermal Energies	-569.86644
Sum of electronic and thermal Enthalpies	-569.86549
Sum of electr. and thermal Free Energies	-569.91170
Electronic Energy (BLYP/6-311+G**)	-570.16402

37. 48e to 48p (48t)

Electronic Energy (BLYP/6-31G*)	-385.49415
Sum of electronic and zero-point Energies	-385.35885
Sum of electronic and thermal Energies	-385.35029
Sum of electronic and thermal Enthalpies	-385.34934
Sum of electr. and thermal Free Energies	-385.39206
Electronic Energy (BLYP/6-311+G**)	-385.60560

38. 49e to 49p (49t)

Electronic Energy (BLYP/6-31G*)	-362.28463
Sum of electronic and zero-point Energies	-362.18793
Sum of electronic and thermal Energies	-362.18075
Sum of electronic and thermal Enthalpies	-362.17981
Sum of electr. and thermal Free Energies	-362.21892
Electronic Energy (BLYP/6-311+G**)	-362.39311

39. 50e to 50p (50t)

Electronic Energy (BLYP/6-31G*)	-362.28400
Sum of electronic and zero-point Energies	-362.18706
Sum of electronic and thermal Energies	-362.18002
Sum of electronic and thermal Enthalpies	-362.17907
Sum of electr. and thermal Free Energies	-362.21785
Electronic Energy (BLYP/6-311+G**)	-362.39229

40. 51e to 51p (51t)

Electronic Energy (BLYP/6-31G*)	-378.32634
Sum of electronic and zero-point Energies	-378.24070
Sum of electronic and thermal Energies	-378.23387
Sum of electronic and thermal Enthalpies	-378.23292
Sum of electr. and thermal Free Energies	-378.27145
Electronic Energy (BLYP/6-311+G**)	-378.43749

41. 52e to 52p (52t)

Electronic Energy (BLYP/6-31G*)	-378.34228
Sum of electronic and zero-point Energies	-378.25703
Sum of electronic and thermal Energies	-378.25011
Sum of electronic and thermal Enthalpies	-378.24917
Sum of electr. and thermal Free Energies	-378.28789
Electronic Energy (BLYP/6-311+G**)	-378.45454

42. 53e to 53p (53t)

Electronic Energy (BLYP/6-31G*)	-378.71228
Sum of electronic and zero-point Energies	-378.61312
Sum of electronic and thermal Energies	-378.60630
Sum of electronic and thermal Enthalpies	-378.60536
Sum of electr. and thermal Free Energies	-378.64385
Electronic Energy (BLYP/6-311+G**)	-378.81571

43. 54e to 54p (54t)

Electronic Energy (BLYP/6-31G*)	-308.09796
Sum of electronic and zero-point Energies	-307.99648
Sum of electronic and thermal Energies	-307.98966
Sum of electronic and thermal Enthalpies	-307.98871
Sum of electr. and thermal Free Energies	-308.02706
Electronic Energy (BLYP/6-311+G**)	-308.18678

44. 54mr to 54p (54ot)

Electronic Energy (BLYP/6-31G*)	-308.12746
Sum of electronic and zero-point Energies	-308.02356
Sum of electronic and thermal Energies	-308.01728
Sum of electronic and thermal Enthalpies	-308.01633
Sum of electr. and thermal Free Energies	-308.05374
Electronic Energy (BLYP/6-311+G**)	-308.21322

III. SINGLET *p*-BENZYNES.

A. Broken Symmetry Optimizations (31 structures)

1. *p*-Benzyne (1p)

Electronic Energy (UBLYP/6-31G*)	-230.77789
Sum of electronic and zero-point Energies	-230.70651
Sum of electronic and thermal Energies	-230.70199
Sum of electronic and thermal Enthalpies	-230.70104
Sum of electr. and thermal Free Energies	-230.73390
Electronic Energy (UBLYP/6-311+G**)	-230.84356

2. 2-Methyl-*p*-benzyne (26p)

Electronic Energy (UBLYP/6-31G*)	-270.06875
Sum of electronic and zero-point Energies	-269.97024
Sum of electronic and thermal Energies	-269.96390
Sum of electronic and thermal Enthalpies	-269.96295
Sum of electr. and thermal Free Energies	-270.00059
Electronic Energy (UBLYP/6-311+G**)	-270.14514

3. 2-Formyl-*p*-benzyne (27p)

Electronic Energy (UBLYP/6-31G*)	-344.08327
Sum of electronic and zero-point Energies	-344.00296
Sum of electronic and thermal Energies	-343.99645
Sum of electronic and thermal Enthalpies	-343.99551
Sum of electr. and thermal Free Energies	-344.03366
Electronic Energy (UBLYP/6-311+G**)	-344.18395

4. 2-Chloro-*p*-benzyne (21p)

Electronic Energy (UBLYP/6-31G*)	-690.35896
Sum of electronic and zero-point Energies	-690.29669
Sum of electronic and thermal Energies	-690.29099
Sum of electronic and thermal Enthalpies	-690.29005
Sum of electr. and thermal Free Energies	-690.32656
Electronic Energy (UBLYP/6-311+G**)	-690.45254

5. 2,3-Dichloro-*p*-benzyne (22p)

Electronic Energy (UBLYP/6-31G*)	-1149.93650
Sum of electronic and zero-point Energies	-1149.88338
Sum of electronic and thermal Energies	-1149.87645
Sum of electronic and thermal Enthalpies	-1149.87551
Sum of electr. and thermal Free Energies	-1149.91555
Electronic Energy (UBLYP/6-311+G**)	-1150.05840

6. 2-Fluoro-*p*-benzyne (19p)

Electronic Energy (UBLYP/6-31G*)	-330.00504
Sum of electronic and zero-point Energies	-329.94146
Sum of electronic and thermal Energies	-329.93611
Sum of electronic and thermal Enthalpies	-329.93517
Sum of electr. and thermal Free Energies	-329.97033
Electronic Energy (UBLYP/6-311+G**)	-330.10796

7. 2,3-Difluoro-*p*-benzyne (20p)

Electronic Energy (UBLYP/6-31G*)	-429.22651
Sum of electronic and zero-point Energies	-429.17065
Sum of electronic and thermal Energies	-429.16438
Sum of electronic and thermal Enthalpies	-429.16343
Sum of electr. and thermal Free Energies	-429.20100
Electronic Energy (UBLYP/6-311+G**)	-429.36688

8. 2-Hydroxy-*p*-benzyne (29p)

Electronic Energy (UBLYP/6-31G*)	-305.98549
Sum of electronic and zero-point Energies	-305.91021

Sum of electronic and thermal Energies	-305.90447
Sum of electronic and thermal Enthalpies	-305.90352
Sum of electr. and thermal Free Energies	-305.93924
Electronic Energy (UBLYP/6-311+G**)	-306.08389

9. 2-Formatoyl-*p*-benzyne (30p)

Electronic Energy (UBLYP/6-31G*)	-419.30371
Sum of electronic and zero-point Energies	-419.21954
Sum of electronic and thermal Energies	-419.21186
Sum of electronic and thermal Enthalpies	-419.21091
Sum of electr. and thermal Free Energies	-419.25241
Electronic Energy (UBLYP/6-311+G**)	-419.42926

10. 2-Amino-*p*-benzyne: pyramidal NH₂ (31p)

Electronic Energy (UBLYP/6-31G*)	-286.11287
Sum of electronic and zero-point Energies	-286.02528
Sum of electronic and thermal Energies	-286.01924
Sum of electronic and thermal Enthalpies	-286.01829
Sum of electr. and thermal Free Energies	-286.05452
Electronic Energy (UBLYP/6-311+G**)	-286.20321

11. 2-Formamido-*p*-benzyne (34p)

Electronic Energy (UBLYP/6-31G*)	-399.43850
Sum of electronic and zero-point Energies	-399.34151
Sum of electronic and thermal Energies	-399.33371
Sum of electronic and thermal Enthalpies	-399.33276
Sum of electr. and thermal Free Energies	-399.37415
Electronic Energy (UBLYP/6-311+G**)	-399.56063

12. 2,3-Cyclopentano-*p*-benzyne (23p)

Electronic Energy (UBLYP/6-31G*)	-347.44975
Sum of electronic and zero-point Energies	-347.31548
Sum of electronic and thermal Energies	-347.30843
Sum of electronic and thermal Enthalpies	-347.30748
Sum of electr. and thermal Free Energies	-347.34665
Electronic Energy (UBLYP/6-311+G**)	-347.54431

13. 2-Borohydrido-*p*-benzyne (38p)

Electronic Energy (UBLYP/6-31G*)	-256.83777
Sum of electronic and zero-point Energies	-256.74922
Sum of electronic and thermal Energies	-256.74249
Sum of electronic and thermal Enthalpies	-256.74155
Sum of electr. and thermal Free Energies	-256.77966
Electronic Energy (UBLYP/6-311+G**)	-256.92640

14. 2-Nitro-*p*-benzyne (28p)

Electronic Energy (UBLYP/6-31G*)	-435.27167
Sum of electronic and zero-point Energies	-435.19820
Sum of electronic and thermal Energies	-435.19114
Sum of electronic and thermal Enthalpies	-435.19019
Sum of electr. and thermal Free Energies	-435.23019

Electronic Energy (UBLYP/6-311+G**)	-435.40201
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15. 2-Borano-*p*-benzyne (coplanar) (36p)

Electronic Energy (UBLYP/6-31G*)	-256.20246
Sum of electronic and zero-point Energies	-256.12002
Sum of electronic and thermal Energies	-256.11392
Sum of electronic and thermal Enthalpies	-256.11298
Sum of electr. and thermal Free Energies	-256.14937
Electronic Energy (UBLYP/6-311+G**)	-256.27088

16. 2-Thiohydroxy-*p*-benzyne (39p)

Electronic Energy (UBLYP/6-31G*)	-628.94674
Sum of electronic and zero-point Energies	-628.87639
Sum of electronic and thermal Energies	-628.86995
Sum of electronic and thermal Enthalpies	-628.86900
Sum of electr. and thermal Free Energies	-628.90692
Electronic Energy (UBLYP/6-311+G**)	-629.04302

17. 2-Ammonio-*p*-benzyne (35p)

Electronic Energy (UBLYP/6-31G*)	-286.45890
Sum of electronic and zero-point Energies	-286.35734
Sum of electronic and thermal Energies	-286.35095
Sum of electronic and thermal Enthalpies	-286.35001
Sum of electr. and thermal Free Energies	-286.38772
Electronic Energy (UBLYP/6-311+G**)	-286.53945

18. 9,10-Anthracyne (59)

Electronic Energy (UBLYP/6-31G*)	-537.93156
Sum of electronic and zero-point Energies	-537.76867
Sum of electronic and thermal Energies	-537.75885
Sum of electronic and thermal Enthalpies	-537.75790
Sum of electr. and thermal Free Energies	-537.80375
Electronic Energy (UBLYP/6-311+G**)	-538.06938

19. 1,4-Naphthalene (9p)

Electronic Energy (UBLYP/6-31G*)	-384.35780
Sum of electronic and zero-point Energies	-384.24057
Sum of electronic and thermal Energies	-384.23350
Sum of electronic and thermal Enthalpies	-384.23256
Sum of electr. and thermal Free Energies	-384.27188
Electronic Energy (UBLYP/6-311+G**)	-384.45958

20. Pyridino-*p*-benzyne (10p)

Electronic Energy (UBLYP/6-31G*)	-400.40636
Sum of electronic and zero-point Energies	-400.30107
Sum of electronic and thermal Energies	-400.29412
Sum of electronic and thermal Enthalpies	-400.29318
Sum of electr. and thermal Free Energies	-400.33235
Electronic Energy (UBLYP/6-311+G**)	-400.51212

21. Pyrazino-*p*-benzyne (47p)

Electronic Energy (UBLYP/6-31G*)	-416.45164
Sum of electronic and zero-point Energies	-416.35871
Sum of electronic and thermal Energies	-416.35181
Sum of electronic and thermal Enthalpies	-416.35087
Sum of electr. and thermal Free Energies	-416.39002
Electronic Energy (UBLYP/6-311+G**)	-416.56124

22. Pyrimidino-*p*-benzyne (46p)

Electronic Energy (UBLYP/6-31G*)	-416.45762
Sum of electronic and zero-point Energies	-416.36398
Sum of electronic and thermal Energies	-416.35713
Sum of electronic and thermal Enthalpies	-416.35619
Sum of electr. and thermal Free Energies	-416.39526
Electronic Energy (UBLYP/6-311+G**)	-416.56732

23. Quinoxalino-*p*-benzyne (11p)

Electronic Energy (UBLYP/6-31G*)	-570.03036
Sum of electronic and zero-point Energies	-569.89262
Sum of electronic and thermal Energies	-569.88291
Sum of electronic and thermal Enthalpies	-569.88197
Sum of electr. and thermal Free Energies	-569.92758
Electronic Energy (UBLYP/6-311+G**)	-570.17730

24. 1,4-Cyclohexadieno-*p*-benzyne (48p)

Electronic Energy (UBLYP/6-31G*)	-385.52372
Sum of electronic and zero-point Energies	-385.38481
Sum of electronic and thermal Energies	-385.37683
Sum of electronic and thermal Enthalpies	-385.37588
Sum of electr. and thermal Free Energies	-385.41791
Electronic Energy (UBLYP/6-311+G**)	-385.62916

25. α -Pyrrolo-*p*-benzyne (49p)

Electronic Energy (UBLYP/6-31G*)	-362.30573
Sum of electronic and zero-point Energies	-362.20616
Sum of electronic and thermal Energies	-362.19951
Sum of electronic and thermal Enthalpies	-362.19856
Sum of electr. and thermal Free Energies	-362.23667
Electronic Energy (UBLYP/6-311+G**)	-362.40862

26. β -Pyrrolo-*p*-benzyne (50p)

Electronic Energy (UBLYP/6-31G*)	-362.29787
Sum of electronic and zero-point Energies	-362.19878
Sum of electronic and thermal Energies	-362.19209
Sum of electronic and thermal Enthalpies	-362.19115
Sum of electr. and thermal Free Energies	-362.22923
Electronic Energy (UBLYP/6-311+G**)	-362.40132

27. Isoimidazolo-*p*-benzyne (51p)

Electronic Energy (UBLYP/6-31G*)	-378.34557
Sum of electronic and zero-point Energies	-378.25738
Sum of electronic and thermal Energies	-378.25095

Sum of electronic and thermal Enthalpies	-378.25000
Sum of electr. and thermal Free Energies	-378.28778
Electronic Energy (UBLYP/6-311+G**)	-378.45142

28. Imidazolo-*p*-benzyne (52p)

Electronic Energy (UBLYP/6-31G*)	-378.36580
Sum of electronic and zero-point Energies	-378.27748
Sum of electronic and thermal Energies	-378.27114
Sum of electronic and thermal Enthalpies	-378.27020
Sum of electr. and thermal Free Energies	-378.30778
Electronic Energy (UBLYP/6-311+G**)	-378.47240

29. Imidazolium-*p*-benzyne (53p)

Electronic Energy (UBLYP/6-31G*)	-378.73330
Sum of electronic and zero-point Energies	-378.63111
Sum of electronic and thermal Energies	-378.62476
Sum of electronic and thermal Enthalpies	-378.62382
Sum of electr. and thermal Free Energies	-378.66142
Electronic Energy (UBLYP/6-311+G**)	-378.83214

30. Cyclobutano-*p*-benzyne (54p)

Electronic Energy (UBLYP/6-31G*)	-308.12957
Sum of electronic and zero-point Energies	-308.02527
Sum of electronic and thermal Energies	-308.01897
Sum of electronic and thermal Enthalpies	-308.01803
Sum of electr. and thermal Free Energies	-308.05533
Electronic Energy (UBLYP/6-311+G**)	-308.21307

31. 2-Borano-*p*-benzyne (perpendicular) (37p)

(this case not fully opted; off by 1.1D-09 Hartrees)

Electronic Energy (UBLYP/6-31G*)	-256.18820
Electronic Energy (UBLYP/6-311+G**)	-256.25738

B. Restricted Optimizations (8 structures)**1. 2-Amino-*p*-benzyne: planar/coplanar NH₂ (32p)**

Electronic Energy (BLYP/6-31G*)	-286.10049
Sum of electronic and zero-point Energies	-286.01562
Sum of electronic and thermal Energies	-286.00997
Sum of electronic and thermal Enthalpies	-286.00903
Sum of electr. and thermal Free Energies	-286.04460
Electronic Energy (BLYP/6-311+G**)	-286.19371
Electronic Energy (UBLYP/6-31G*)	-286.10721
Electronic Energy (UBLYP/6-311+G**)	-286.19371

2. 2-Amino-*p*-benzyne: planar/perpendicular NH₂ (33p)

Electronic Energy (BLYP/6-31G*)	-286.08860
Sum of electronic and zero-point Energies	-286.00384
Sum of electronic and thermal Energies	-285.99829
Sum of electronic and thermal Enthalpies	-285.99734
Sum of electr. and thermal Free Energies	-286.03281

Electronic Energy (BLYP/6-311+G**)	-286.18184
Electronic Energy (UBLYP/6-31G*)	-286.09298
Electronic Energy (UBLYP/6-311+G**)	-286.18558

3. 2-Sulfoxyl-*p*-benzyne (40p)

Electronic Energy (BLYP/6-31G*)	-704.09652
Sum of electronic and zero-point Energies	-704.02292
Sum of electronic and thermal Energies	-704.01552
Sum of electronic and thermal Enthalpies	-704.01457
Sum of electr. and thermal Free Energies	-704.05572
Electronic Energy (BLYP/6-311+G**)	-704.22171
Electronic Energy (UBLYP/6-31G*)	-704.10129
Electronic Energy (UBLYP/6-311+G**)	-704.22171

4. 2-Phenyl-*p*-benzyne (41p)

Electronic Energy (BLYP/6-31G*)	-461.72271
Sum of electronic and zero-point Energies	-461.57369
Sum of electronic and thermal Energies	-461.56423
Sum of electronic and thermal Enthalpies	-461.56329
Sum of electr. and thermal Free Energies	-461.60881
Electronic Energy (BLYP/6-311+G**)	-461.84807
Electronic Energy (UBLYP/6-31G*)	-461.72847
Electronic Energy (UBLYP/6-311+G**)	-461.85289

5. 2-(*p*-Fluorophenyl)-*p*-benzyne (42p)

Electronic Energy (BLYP/6-31G*)	-560.95604
Sum of electronic and zero-point Energies	-560.81516
Sum of electronic and thermal Energies	-560.80482
Sum of electronic and thermal Enthalpies	-560.80388
Sum of electr. and thermal Free Energies	-560.85160
Electronic Energy (BLYP/6-311+G**)	-561.11934
Electronic Energy (UBLYP/6-31G*)	-560.96175
Electronic Energy (UBLYP/6-311+G**)	-561.12420

6. 2-(*p*-Boranophenyl)-*p*-benzyne (43p)

Electronic Energy (BLYP/6-31G*)	-487.14499
Sum of electronic and zero-point Energies	-486.98490
Sum of electronic and thermal Energies	-486.97386
Sum of electronic and thermal Enthalpies	-486.97292
Sum of electr. and thermal Free Energies	-487.02183
Electronic Energy (BLYP/6-311+G**)	-487.27279
Electronic Energy (UBLYP/6-31G*)	-487.15079
Electronic Energy (UBLYP/6-311+G**)	-487.27776

7. Cyclohexano-*p*-benzyne (17p)

Electronic Energy (BLYP/6-31G*)	-386.72718
Sum of electronic and zero-point Energies	-386.56532
Sum of electronic and thermal Energies	-386.55690
Sum of electronic and thermal Enthalpies	-386.55596
Sum of electr. and thermal Free Energies	-386.59829
Electronic Energy (BLYP/6-311+G**)	-386.83446

Electronic Energy (UBLYP/6-31G*)	-386.73378
Electronic Energy (UBLYP/6-311+G**)	-386.84002

8. 2-Chloro-5,6-cyclohexano-*p*-benzyne (13p)

Electronic Energy (BLYP/6-31G*)	-846.30544
Sum of electronic and zero-point Energies	-846.15329
Sum of electronic and thermal Energies	-846.14419
Sum of electronic and thermal Enthalpies	-846.14325
Sum of electr. and thermal Free Energies	-846.18792
Electronic Energy (BLYP/6-311+G**)	-846.44048
Electronic Energy (UBLYP/6-31G*)	-846.31459
Electronic Energy (UBLYP/6-311+G**)	-846.44867

IV. TRIPLET *p*-BENZYNES (28 structures).1. triplet *p*-Benzyne (³1p)

Electronic Energy (UBLYP/6-31G*)	-230.77139
Sum of electronic and zero-point Energies	-230.69923
Sum of electronic and thermal Energies	-230.69472
Sum of electronic and thermal Enthalpies	-230.69377
Sum of electr. and thermal Free Energies	-230.72638
Electronic Energy (UBLYP/6-311+G**)	-230.83630

2. triplet 2-Methyl-*p*-benzyne (³26p)

Electronic Energy (UBLYP/6-31G*)	-270.06268
Sum of electronic and zero-point Energies	-269.96358
Sum of electronic and thermal Energies	-269.95808
Sum of electronic and thermal Enthalpies	-269.95713
Sum of electr. and thermal Free Energies	-269.99362
Electronic Energy (UBLYP/6-311+G**)	-270.13852

3. triplet 2-Chloro-*p*-benzyne (³21p)

Electronic Energy (UBLYP/6-31G*)	-690.35552
Sum of electronic and zero-point Energies	-690.29269
Sum of electronic and thermal Energies	-690.28700
Sum of electronic and thermal Enthalpies	-690.28606
Sum of electr. and thermal Free Energies	-690.32363
Electronic Energy (UBLYP/6-311+G**)	-690.44874

4. triplet 2,3-Dichloro-*p*-benzyne (³22p)

Electronic Energy (UBLYP/6-31G*)	-1149.93560
Sum of electronic and zero-point Energies	-1149.88215
Sum of electronic and thermal Energies	-1149.87523
Sum of electronic and thermal Enthalpies	-1149.87429
Sum of electr. and thermal Free Energies	-1149.91540
Electronic Energy (UBLYP/6-311+G**)	-1150.05748

5. triplet 2-Fluoro-*p*-benzyne (³19p)

Electronic Energy (UBLYP/6-31G*)	-330.00167
Sum of electronic and zero-point Energies	-329.93742

Sum of electronic and thermal Energies	-329.93212
Sum of electronic and thermal Enthalpies	-329.93117
Sum of electr. and thermal Free Energies	-329.96735
Electronic Energy (UBLYP/6-311+G**)	-330.10449

6. triplet 2,3-Difluoro-*p*-benzyne (³20p)

Electronic Energy (UBLYP/6-31G*)	-429.22578
Sum of electronic and zero-point Energies	-429.16947
Sum of electronic and thermal Energies	-429.16325
Sum of electronic and thermal Enthalpies	-429.16230
Sum of electr. and thermal Free Energies	-429.20086
Electronic Energy (UBLYP/6-311+G**)	-429.36646

7. triplet 2-Hydroxy-*p*-benzyne (³29p)

Electronic Energy (UBLYP/6-31G*)	-305.98163
Sum of electronic and zero-point Energies	-305.90556
Sum of electronic and thermal Energies	-305.89990
Sum of electronic and thermal Enthalpies	-305.89896
Sum of electr. and thermal Free Energies	-305.93562
Electronic Energy (UBLYP/6-311+G**)	-306.07953

8. triplet 2-Amino-*p*-benzyne: pyramidal NH₂ (³31p)

Electronic Energy (UBLYP/6-31G*)	-286.10835
Sum of electronic and zero-point Energies	-286.01999
Sum of electronic and thermal Energies	-286.01401
Sum of electronic and thermal Enthalpies	-286.01307
Sum of electr. and thermal Free Energies	-286.05026
Electronic Energy (UBLYP/6-311+G**)	-286.19818

9. triplet 2,3-Cyclopentano-*p*-benzyne (³23p)

Electronic Energy (UBLYP/6-31G*)	-347.44061
Sum of electronic and zero-point Energies	-347.30552
Sum of electronic and thermal Energies	-347.29849
Sum of electronic and thermal Enthalpies	-347.29754
Sum of electr. and thermal Free Energies	-347.33776
Electronic Energy (UBLYP/6-311+G**)	-347.53462

10. triplet 2-Borohydrido-*p*-benzyne (³38p)

Electronic Energy (UBLYP/6-31G*)	-256.82532
Sum of electronic and zero-point Energies	-256.73587
Sum of electronic and thermal Energies	-256.72909
Sum of electronic and thermal Enthalpies	-256.72814
Sum of electr. and thermal Free Energies	-256.76892
Electronic Energy (UBLYP/6-311+G**)	-256.91266

11. triplet 2-Nitro-*p*-benzyne (³28p)

Electronic Energy (UBLYP/6-31G*)	-435.26822
Sum of electronic and zero-point Energies	-435.19418
Sum of electronic and thermal Energies	-435.18712
Sum of electronic and thermal Enthalpies	-435.18618
Sum of electr. and thermal Free Energies	-435.22717

Electronic Energy (UBLYP/6-311+G**)	-435.39825
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12. triplet 2-Borano-*p*-benzyne (³36p)

Electronic Energy (UBLYP/6-31G*)	-256.19387
Sum of electronic and zero-point Energies	-256.11070
Sum of electronic and thermal Energies	-256.10458
Sum of electronic and thermal Enthalpies	-256.10364
Sum of electr. and thermal Free Energies	-256.14117
Electronic Energy (UBLYP/6-311+G**)	-256.26162

13. triplet 2-Thiohydroxy-*p*-benzyne (³39p)

Electronic Energy (UBLYP/6-31G*)	-628.94201
Sum of electronic and zero-point Energies	-628.87100
Sum of electronic and thermal Energies	-628.86458
Sum of electronic and thermal Enthalpies	-628.86364
Sum of electr. and thermal Free Energies	-628.90257
Electronic Energy (UBLYP/6-311+G**)	-629.03772

14. triplet 2-Sulfoxyl-*p*-benzyne (³40p)

Electronic Energy (UBLYP/6-31G*)	-704.09991
Sum of electronic and zero-point Energies	-704.02516
Sum of electronic and thermal Energies	-704.01787
Sum of electronic and thermal Enthalpies	-704.01693
Sum of electr. and thermal Free Energies	-704.05876
Electronic Energy (UBLYP/6-311+G**)	-704.22398

15. triplet 2-Ammonio-*p*-benzyne (³35p)

Electronic Energy (UBLYP/6-31G*)	-286.45547
Sum of electronic and zero-point Energies	-286.35332
Sum of electronic and thermal Energies	-286.34697
Sum of electronic and thermal Enthalpies	-286.34603
Sum of electr. and thermal Free Energies	-286.38456
Electronic Energy (UBLYP/6-311+G**)	-286.53563

16. triplet 9,10-Anthracyne (³59)

Electronic Energy (UBLYP/6-31G*)	-537.92394
Sum of electronic and zero-point Energies	-537.76023
Sum of electronic and thermal Energies	-537.75046
Sum of electronic and thermal Enthalpies	-537.74952
Sum of electr. and thermal Free Energies	-537.79641
Electronic Energy (UBLYP/6-311+G**)	-538.06187

17. triplet 1,4-Naphthalene (³9p)

Electronic Energy (UBLYP/6-31G*)	-384.35048
Sum of electronic and zero-point Energies	-384.23243
Sum of electronic and thermal Energies	-384.22540
Sum of electronic and thermal Enthalpies	-384.22445
Sum of electr. and thermal Free Energies	-384.26481
Electronic Energy (UBLYP/6-311+G**)	-384.45191

18. triplet Pyrido-*p*-benzyne (³10p)

Electronic Energy (UBLYP/6-31G*)	-400.39902
Sum of electronic and zero-point Energies	-400.29271
Sum of electronic and thermal Energies	-400.28581
Sum of electronic and thermal Enthalpies	-400.28487
Sum of electr. and thermal Free Energies	-400.32505
Electronic Energy (UBLYP/6-311+G**)	-400.50464

19. triplet Pyrazino-*p*-benzynes (³47p)

Electronic Energy (UBLYP/6-31G*)	-416.44370
Sum of electronic and zero-point Energies	-416.34940
Sum of electronic and thermal Energies	-416.34261
Sum of electronic and thermal Enthalpies	-416.34166
Sum of electr. and thermal Free Energies	-416.38173
Electronic Energy (UBLYP/6-311+G**)	-416.55338

20. triplet Pyrimidino-*p*-benzynes (³46p)

Electronic Energy (UBLYP/6-31G*)	-416.44910
Sum of electronic and zero-point Energies	-416.35439
Sum of electronic and thermal Energies	-416.34758
Sum of electronic and thermal Enthalpies	-416.34664
Sum of electr. and thermal Free Energies	-416.38674
Electronic Energy (UBLYP/6-311+G**)	-416.55870

21. triplet Quinoxalino-*p*-benzynes (³11p)

Electronic Energy (UBLYP/6-31G*)	-570.02134
Sum of electronic and zero-point Energies	-569.88189
Sum of electronic and thermal Energies	-569.87240
Sum of electronic and thermal Enthalpies	-569.87146
Sum of electr. and thermal Free Energies	-569.91782
Electronic Energy (UBLYP/6-311+G**)	-570.16834

22. triplet β-Pyrrolo-*p*-benzynes (³50p)

Electronic Energy (UBLYP/6-31G*)	-362.28439
Sum of electronic and zero-point Energies	-362.18380
Sum of electronic and thermal Energies	-362.17730
Sum of electronic and thermal Enthalpies	-362.17635
Sum of electr. and thermal Free Energies	-362.21525
Electronic Energy (UBLYP/6-311+G**)	-362.38687

23. triplet Imidazolium-*p*-benzynes (³53p)

Electronic Energy (UBLYP/6-31G*)	-378.72639
Sum of electronic and zero-point Energies	-378.62343
Sum of electronic and thermal Energies	-378.61712
Sum of electronic and thermal Enthalpies	-378.61617
Sum of electr. and thermal Free Energies	-378.65479
Electronic Energy (UBLYP/6-311+G**)	-378.82492

24. triplet Cyclobutano-*p*-benzynes (³54p)

Electronic Energy (UBLYP/6-31G*)	-308.11207
Sum of electronic and zero-point Energies	-308.00618
Sum of electronic and thermal Energies	-308.00007

Sum of electronic and thermal Enthalpies	-307.99912
Sum of electr. and thermal Free Energies	-308.03712
Electronic Energy (UBLYP/6-311+G**)	-308.19431

25. triplet Isoimidazolo-*p*-benzynes (³51p)

Electronic Energy (UBLYP/6-31G*)	-378.33477
Sum of electronic and zero-point Energies	-378.24549
Sum of electronic and thermal Energies	-378.23912
Sum of electronic and thermal Enthalpies	-378.23818
Sum of electr. and thermal Free Energies	-378.27693
Electronic Energy (UBLYP/6-311+G**)	-378.43999

26. triplet 1,4-Cyclohexadieno-*p*-benzynes (³48p)

Electronic Energy (UBLYP/6-31G*)	-385.51872
Sum of electronic and zero-point Energies	-385.37917
Sum of electronic and thermal Energies	-385.37124
Sum of electronic and thermal Enthalpies	-385.37029
Sum of electr. and thermal Free Energies	-385.41314
Electronic Energy (UBLYP/6-311+G**)	-385.62386

27. triplet α-Pyrrolo-*p*-benzynes (³49p)

Electronic Energy (UBLYP/6-31G*)	-362.29581
Sum of electronic and zero-point Energies	-362.19514
Sum of electronic and thermal Energies	-362.18857
Sum of electronic and thermal Enthalpies	-362.18763
Sum of electr. and thermal Free Energies	-362.22667
Electronic Energy (UBLYP/6-311+G**)	-362.39804

28. triplet Imidazolo-*p*-benzynes (³52p)

Electronic Energy (UBLYP/6-31G*)	-378.35526
Sum of electronic and zero-point Energies	-378.26583
Sum of electronic and thermal Energies	-378.25956
Sum of electronic and thermal Enthalpies	-378.25861
Sum of electr. and thermal Free Energies	-378.29716
Electronic Energy (UBLYP/6-311+G**)	-378.46146

V. ADDITIONAL RELATED COMPOUNDS (21 structures).

A. Radicals (9 structures)

1. Phenyl

Electronic Energy (BLYP/6-31G*)	-231.45321
Sum of electronic and zero-point Energies	-231.36834
Sum of electronic and thermal Energies	-231.36384
Sum of electronic and thermal Enthalpies	-231.36289
Sum of electr. and thermal Free Energies	-231.39646
Electronic Energy (UBLYP/6-311+G**)	-231.51980

2. 2,3-Difluorophenyl

Electronic Energy (BLYP/6-31G*) -429.90998
 Sum of electronic and zero-point Energies -429.84107
 Sum of electronic and thermal Energies -429.83487
 Sum of electronic and thermal Enthalpies -429.83392
 Sum of electr. and thermal Free Energies -429.87203

Electronic Energy (UBLYP/6-311+G**) -430.05223

3. α -Naphthyl

Electronic Energy (BLYP/6-31G*) -385.03244
 Sum of electronic and zero-point Energies -384.90179
 Sum of electronic and thermal Energies -384.89477
 Sum of electronic and thermal Enthalpies -384.89383
 Sum of electr. and thermal Free Energies -384.93377
 Electronic Energy (UBLYP/6-311+G**) -385.13522

4. α -Indanyl

Electronic Energy (BLYP/6-31G*) -348.12230
 Sum of electronic and zero-point Energies -347.97473
 Sum of electronic and thermal Energies -347.96771
 Sum of electronic and thermal Enthalpies -347.96676
 Sum of electr. and thermal Free Energies -348.00658

Electronic Energy (UBLYP/6-311+G**) -348.21755

5. α -Cyclobutaphenyl

Electronic Energy (BLYP/6-31G*) -308.79545
 Sum of electronic and zero-point Energies -308.67718
 Sum of electronic and thermal Energies -308.67107
 Sum of electronic and thermal Enthalpies -308.67012
 Sum of electr. and thermal Free Energies -308.70774
 Electronic Energy (UBLYP/6-311+G**) -308.87900

6. α -Quinoxalyl

Electronic Energy (BLYP/6-31G*) -570.70519
 Sum of electronic and zero-point Energies -570.55303
 Sum of electronic and thermal Energies -570.54357
 Sum of electronic and thermal Enthalpies -570.54263
 Sum of electr. and thermal Free Energies -570.58852
 Electronic Energy (UBLYP/6-311+G**) -570.85365

7. 9-Anthryl

Electronic Energy (BLYP/6-31G*) -538.60607
 Sum of electronic and zero-point Energies -538.42993
 Sum of electronic and thermal Energies -538.42019
 Sum of electronic and thermal Enthalpies -538.41925
 Sum of electr. and thermal Free Energies -538.46560

Electronic Energy (UBLYP/6-311+G**) -538.74511

8. α -Isopyrrolophenyl

Electronic Energy (BLYP/6-31G*) -362.96690
 Sum of electronic and zero-point Energies -362.85383
 Sum of electronic and thermal Energies -362.84734
 Sum of electronic and thermal Enthalpies -362.84639
 Sum of electr. and thermal Free Energies -362.88488

Electronic Energy (UBLYP/6-311+G**) -363.07079

9. α -Imidazoliumphenyl

Electronic Energy (BLYP/6-31G*) -379.41472
 Sum of electronic and zero-point Energies -379.29915
 Sum of electronic and thermal Energies -379.29283
 Sum of electronic and thermal Enthalpies -379.29189
 Sum of electr. and thermal Free Energies -379.33013
 Electronic Energy (UBLYP/6-311+G**) -379.51491

B. Arenes (9 structures)

1. Benzene

Electronic Energy (BLYP/6-31G*) -232.13234
 Sum of electronic and zero-point Energies -232.03458
 Sum of electronic and thermal Energies -232.03007
 Sum of electronic and thermal Enthalpies -232.02913
 Sum of electr. and thermal Free Energies -232.06211

2. o-Difluorobenzene

Electronic Energy (BLYP/6-31G*) -430.59292
 Sum of electronic and zero-point Energies -430.51126
 Sum of electronic and thermal Energies -430.50509
 Sum of electronic and thermal Enthalpies -430.50414
 Sum of electr. and thermal Free Energies -430.54154

3. Naphthalene

Electronic Energy (BLYP/6-31G*) -385.71175
 Sum of electronic and zero-point Energies -385.56835
 Sum of electronic and thermal Energies -385.56134
 Sum of electronic and thermal Enthalpies -385.56039
 Sum of electr. and thermal Free Energies -385.59969

4. Indan

Electronic Energy (BLYP/6-31G*) -348.80073
 Sum of electronic and zero-point Energies -348.64052
 Sum of electronic and thermal Energies -348.63348
 Sum of electronic and thermal Enthalpies -348.63253
 Sum of electr. and thermal Free Energies -348.67173

5. Cyclobutabenzene

Electronic Energy (BLYP/6-31G*) -309.47369
 Sum of electronic and zero-point Energies -309.34279
 Sum of electronic and thermal Energies -309.33665
 Sum of electronic and thermal Enthalpies -309.33571

Sum of electronic and thermal Free Energies-309.37273

6. Anthracene

Electronic Energy (BLYP/6-31G*)	-539.28553
Sum of electronic and zero-point Energies	-539.09687
Sum of electronic and thermal Energies	-539.08714
Sum of electronic and thermal Enthalpies	-539.08619
Sum of electr. and thermal Free Energies	-539.13182

7. Quinoxaline

Electronic Energy (BLYP/6-31G*)	-571.38604
Sum of electronic and zero-point Energies	-571.22092
Sum of electronic and thermal Energies	-571.21147
Sum of electronic and thermal Enthalpies	-571.21053
Sum of electr. and thermal Free Energies	-571.25572

8. Benzo-isopyrrole ([b,c]benzopyrrole)

Electronic Energy (BLYP/6-31G*)	-363.64546
Sum of electronic and zero-point Energies	-363.51964
Sum of electronic and thermal Energies	-363.51315
Sum of electronic and thermal Enthalpies	-363.51220
Sum of electr. and thermal Free Energies	-363.55005

9. Benzo-imidazolium Ion

Electronic Energy (BLYP/6-31G*)	-380.10042
Sum of electronic and zero-point Energies	-379.97205
Sum of electronic and thermal Energies	-379.96571
Sum of electronic and thermal Enthalpies	-379.96477
Sum of electr. and thermal Free Energies	-380.00240

C. Others (3 structures)

1. 7-H-7,9-Diazacyclodeca-3,7,9-trien-1,5-diyne cation (55)

Electronic Energy (BLYP/6-31G*)	-416.80893
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2. 4,6-Diaza-cyclodeca-1,2,3,5-tetraene-8-yne (56)

Electronic Energy (BLYP/6-31G*)	-417.62800
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3. 3,5-Diaza-cyclodeca-3,5-diene-1,7-diyne (57)

Electronic Energy (BLYP/6-31G*)	-417.63328
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