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Supporting Information

Atom-dispersed Au combined with Nano-Au on Halloysite Nanotubes with Closo-dodecaborate promotes Synergistic Effects for Enhanced Photocatalysis

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Figure S1. FT-IR spectra of $HNT@B_{12}H_{12}@Au(a)$; PXRD spectra of $HNT@B_{12}H_{12}@Au(b)$; XPS spectra of $HNT@B_{12}H_{12}@Au(c, d)$; and XPS spectra of B before (e) and after (f) Au reduction.



Figure S2. TEM of Na₂B₁₂H₁₂@Au.



Figure S3. XPS spectra of HNT@Au.

 $\label{eq:stable} \textbf{Table S1. pH} \ \text{values before and after reaction and the effect of different solvents on the reducibility of $Na_2B_{12}H_{12}$.}$

Entry	$Na_2B_{12}H_{12}$	NaAuCl ₄	Solvent	Time	Solution color	pН
1	-	0.1mmol	H ₂ O(30 mL)	10 min	yellow	3.63
2	0.5mmol	-	$H_2O(30 \text{ mL})$	10 min	colorless	7.02
3	0.5mmol	0.1mmol	H ₂ O(30 mL)	10 min	purple black	3.11
4	0.5mmol	0.1mmol	MeOH(30 mL)	10 min	yellow	-
5	0.5mmol	0.1mmol	EtOH(30 mL)	10 min	yellow	-
6	0.5mmol	0.1mmol	CH ₂ Cl ₂ (30 mL)	10 min	yellow	-
7	0.5mmol	0.1mmol	Acetone(30 mL)	10 min	yellow	-
8	0.5mmol	0.1mmol	DMF(30 mL)	10 min	yellow	-

Table S2. Catalytic effect of different catalysts on different substrates^[a].

Entry	Reactant	Catalyst	Yi	eld(%) of	AOB at	different R	leactin ti	ne ^[b]	Yie	ld(%) of A	AB at di	fferent R	eactin ti	me ^[b]
			0 h	0.5h	1h	1.5h	2h	2.5h	0 h	0.5h	1h	1.5h	2h	2.5h
1	NB	HNT@Au	-	4.0	7.2	9.4	14	12	-	4.2	5.1	5.4	5.8	6.4
2	NB	Na2B12H12@Au	-	10	22	69	40	4.2	-	-	-	15	38	63
3	NB	HNT@B ₁₂ H ₁₂ @Au	-	18	29	48	28	-	-	8.1	12	37	69	97
4	NSB	HNT@Au	-	24	49	58	41	-	-	5.7	9.2	14	19	28
5	NSB	Na ₂ B ₁₂ H ₁₂ @Au	-	9.9	14	31	44	-	-	3.2	8.5	21	39	57
6	NSB	HNT@B12H12@Au	-	31	52	42	28	3.9	-	8.4	17	45	71	98
7	AOB	HNT@Au	-	-	-	-	-	-	-	12	19	24	31	37
8	AOB	Na2B12H12@Au	-	-	-	-	-	-	-	17	29	37	46	54
9	AOB	HNT@B ₁₂ H ₁₂ @Au	-	-	-	-	-	-	-	25	42	68	82	98
[a] Reaction c	ondition:, reactant	0.5 mmol, photocatalyst 0.	5 µmol	(base on A	Au), 5 ml	L 2-propar	nol as sol	vent, 0.75	mmol 1	NaOH as l	base, 1 a	tm N ₂ atı	mospher	e,
room tempera	ture, reaction time	from 0-2.5 h, and the light	(≈370 n	m) intensi	ty was 0	.54 W/cm ²	2. [b] The	conversa	tions we	ere analyz	ed by ga	is chroma	atograph	ıy
(GC).														

 $\label{eq:solution} \textbf{Table S3.} Comparison of HNT@B_{12}H_{12}@Au with reported solid catalysts for the reduction of nitrobenzene to AB.$

Catalyst	Conditions	TON	TOF(h-1)	Ref.
BM-Au/TiO ₂	2-propanol, KOH, visible-light, 12h, R.T.	43.3	3.61	[1]
Cu/graphene	2-propanol, KOH, 400-800 nm, 12 h, 90°C	36.6	3.05	[2]
g-C ₃ N ₄	2-propanol,KOH, 410 nm LED , 5h, R.T.	0.0375	0.0075	[3]
Au@CeO2	2-propanol,KOH, 4h, 50°C	12.4	3.09	[4]
Au@OC1R	2-propanol,KOH, UV, 2h, 30°C	182	91.0	[5]
SmI_2	THF, n-Bu4NPF6, electrical drive, 2h, 20°C	9.50	4.75	[6]
Ag@ZrO ₂	2-propanol,KOH, UV, 2h, 60°C	32.0	2.00	[7]
Na2B12H12@Au	2-propanol,KOH, 370nm, 2.5h, R.T.	7.60	3.10	This work
HNT@B12H12@Au	2-propanol,KOH, 370nm, 2.5h, R.T.	218	87.1	This work



Figure S4. EPR spectra of the Na₂B₁₂H₁₂ reduction of Au NPs from 0 to 60 min; 2, 2-dimethyl-3,4-dihydro-2H-pyrrole 1-oxide (DMPO) was added in each period (0, 1, 2, 3, 4, and 60 min).



Figure S5. LTQ-XL mass spectrometry of $B_{12}H_{12}^{2-}$ before and after reaction (a, b). The detailed m/z after the reaction is shown in (c), and the proposed mechanism for Au-NP synthesis by $B_{12}H_{12}^{2-}$ is summarized in (1–3). The m/z of $B_{12}H_{12}^{2-}$ derivatives are shown in (3) (because the eluent is acetonitrile, 1–2 molecular weights of acetonitrile should be added when calculating the m/z of $B_{12}H_{12}^{2-}$ derivatives).



Figure S6. UV-vis spectrometry of HNT@ $B_{12}H_{12}$ @Au and Na₂ $B_{12}H_{12}$ @Au (a). The photocurrent density (*I*-*t* curves) of different materials under UV radiation at 370 nm wavelength (b).



Figure S7. Effect of irradiation density (power) on reaction (The irradiation density corresponding to 25W is 0.54 W/cm²). Reaction condition: photocatalyst 100 mg, reactant 0.5 mmol, 5 mL 2-propanol as solvent, 0.75 mmol NaOH as base, 1 atm N₂ atmosphere, room temperature, reaction time 2.5 h, and the irradiation ($\lambda \approx 370$ nm), 0, 5, 15, 20, 25 and 30W corresponds to the irradiation density of 0, 0.11, 0.32, 0.54 and 0.65 W/cm².



Figure S8. Isolation yields of azobenzene at different irradiation densities. Reaction condition: photocatalyst 100 mg, reactant 0.5 mmol, 5 mL 2-propanol as solvent, 0.75 mmol NaOH as base, 1 atm N₂ atmosphere, room temperature, reaction time 2.5 h, and the irradiation ($\lambda \approx 370$ nm), 0, 5, 15, 20, 25 and 30W corresponds to the irradiation density of 0, 0.11, 0.32, 0.54 and 0.65 W/cm².



Figure S9. Models of Au-Al-Osite.



Figure S10. Models of Au-B-Al-Osite.



Figure S11. Models of Au-B-Osite.



Figure S12. Models of Au-NP site.



Figure S13. Isodensity contour plot of the Fukui function f (+), f (0), f (-) and delta f for NB.



Figure S14. Isodensity contour plot of the Fukui function f (+), f (0), f (-) and delta f for the nitrosobenzene (NSB).



Figure S15. Isodensity contour plot of the Fukui function f (+), f (0), f (-) and delta f for the di-nitrosobenzene (D-NSB).



Figure S16. Isodensity contour plot of the Fukui function f (+), f (0), f (-) and delta f for the hydrogenated NSB (NSB-H).



Figure S17. Isodensity contour plot of the Fukui function f(+), f(0), f(-) and delta f for the azoxybenzene (AOB).



Figure S18. Isodensity contour plot of the Fukui function f (+), f (0), f (-) and delta f for the azobenzene (AB).

Table S4. Mulliken atomic charges of nitrobenzene (NB), azobenzene (AB) and azoxybenzene (AOB) have been calculated using GGA-PBE.

	Atomic Populatio	ns (Mull	iken) of	NB			
Species	Ion	s	р	d	f	Total	Charge(e)
Н	1	0.67	0.00	0.00	0.00	0.67	0.33
Η	2	0.66	0.00	0.00	0.00	0.66	0.34
Н	3	0.69	0.00	0.00	0.00	0.69	0.31
Н	4	0.69	0.00	0.00	0.00	0.69	0.31
Н	5	0.70	0.00	0.00	0.00	0.70	0.30
С	1	1.26	3.00	0.00	0.00	4.26	-0.26
С	2	1.27	2.99	0.00	0.00	4.26	-0.26
С	3	1.26	3.02	0.00	0.00	4.27	-0.27
С	4	1.26	2.97	0.00	0.00	4.24	-0.24
С	5	1.13	2.76	0.00	0.00	3.89	0.11
С	6	1.26	2.98	0.00	0.00	4.24	-0.24
N	1	1.48	3.28	0.00	0.00	4.76	0.24
0	1	1.94	4.40	0.00	0.00	6.33	-0.33
0	2	1.94	4.39	0.00	0.00	6.33	-0.33
	Atomic Populatio	ns (Mull	iken) of	NSB			
Species	Ion	s	р	d	f	Total	Charge(e)
Н	1	0.76	0.00	0.00	0.00	0.76	0.24
Н	2	0.68	0.00	0.00	0.00	0.68	0.32
Н	3	0.70	0.00	0.00	0.00	0.70	0.30
Н	4	0.70	0.00	0.00	0.00	0.70	0.30
Н	5	0.70	0.00	0.00	0.00	0.70	0.30
Н	6	0.49	0.00	0.00	0.00	0.49	0.51
С	1	1.19	3.09	0.00	0.00	4.27	-0.27
С	2	1.19	3.10	0.00	0.00	4.29	-0.29
С	3	1.19	3.11	0.00	0.00	4.29	-0.29
С	4	1.19	3.08	0.00	0.00	4.27	-0.27
С	5	1.02	2.85	0.00	0.00	3.88	0.12
С	6	1.16	3.16	0.00	0.00	4.33	-0.33
Ν	1	1.64	3.49	0.00	0.00	5.13	-0.13
0	1	1.83	4.68	0.00	0.00	6.51	-0.51
	Atomic Populatio	ns (Mull	iken) of	D-NSB			
Species	Ion	s	р	d	f	Total	Charge(e)
Н	1	0.68	0.00	0.00	0.00	0.68	0.32
Н	2	0.68	0.00	0.00	0.00	0.68	0.32
Н	3	0.70	0.00	0.00	0.00	0.70	0.30
Н	4	0.71	0.00	0.00	0.00	0.71	0.29
Н	5	0.71	0.00	0.00	0.00	0.71	0.29
Н	6	0.69	0.00	0.00	0.00	0.69	0.31
Н	7	0.67	0.00	0.00	0.00	0.67	0.33
Н	8	0.71	0.00	0.00	0.00	0.71	0.29
Н	9	0.71	0.00	0.00	0.00	0.71	0.29
Н	10	0.71	0.00	0.00	0.00	0.71	0.29
С	1	1.26	3.01	0.00	0.00	4.27	-0.27
С	2	1.26	3.01	0.00	0.00	4.27	-0.27
С	3	1.26	3.02	0.00	0.00	4.28	-0.28
С	4	1.26	3.00	0.00	0.00	4.26	-0.26
С	5	1.12	2.76	0.00	0.00	3.88	0.12
С	6	1.25	3.00	0.00	0.00	4.25	-0.25
С	7	1.26	3.01	0.00	0.00	4.27	-0.27

С	8	1 26	3.01	0.00	0.00	4 27	-0.27
Ĉ	9	1.26	3.03	0.00	0.00	4.28	-0.28
c	10	1.20	2.00	0.00	0.00	4.25	-0.28
C	10	1.20	2.99	0.00	0.00	4.25	-0.25
С	11	1.26	3.01	0.00	0.00	3.88	0.12
С	12	1.25	2.99	0.00	0.00	4.25	-0.25
Ν	1	1.41	3.46	0.00	0.00	4.88	0.12
N	2	1 39	3 4 5	0.00	0.00	4 84	0.16
0	1	1.02	1.54	0.00	0.00	6 47	0.10
0	1	1.95	4.54	0.00	0.00	0.47	-0.47
0	2	1.90	4.54	0.00	0.00	6.45	-0.45
	Atomic Populatio	ns (Mull	iken) of	NSB-H			
Species	Ion	s	n	d	f	Total	Charge(e)
11	1	0.69	P	0.00	0.00	0.69	0.22
п	1	0.08	0.00	0.00	0.00	0.08	0.32
Н	2	0.68	0.00	0.00	0.00	0.68	0.32
Н	3	0.69	0.00	0.00	0.00	0.69	0.31
Н	4	0.69	0.00	0.00	0.00	0.69	0.31
Н	5	0.69	0.00	0.00	0.00	0.69	0.31
C	1	1 10	3 10	0.00	0.00	4 29	0.29
c	1	1.19	2.07	0.00	0.00	4.27	-0.29
C	2	1.20	3.07	0.00	0.00	4.27	-0.27
С	3	1.19	3.09	0.00	0.00	4.28	-0.28
С	4	1.19	3.09	0.00	0.00	4.28	-0.28
С	5	1.05	2.83	0.00	0.00	3.88	0.12
С	6	1 19	3.07	0.00	0.00	4 27	-0.27
N	1	1.62	3 36	0.00	0.00	1 98	0.02
N O	1	1.02	3.30	0.00	0.00	4.90	0.02
0	1	1.85	4.46	0.00	0.00	6.31	-0.31
	Atomic Populatio	ns (Mull	iken) of	AOB			
Species	Ion	s	р	d	f	Total	Charge(e)
Н	1	0.68	0.00	0.00	0.00	0.68	0.32
н	- ว	0.60	0.00	0.00	0.00	0.69	0.31
11	2	0.09	0.00	0.00	0.00	0.09	0.31
H	3	0.70	0.00	0.00	0.00	0.70	0.30
Н	4	0.71	0.00	0.00	0.00	0.71	0.29
Н	5	0.71	0.00	0.00	0.00	0.71	0.29
Н	6	0.70	0.00	0.00	0.00	0.70	0.30
н	7	0.67	0.00	0.00	0.00	0.67	0.33
11	,	0.07	0.00	0.00	0.00	0.07	0.35
п	0	0.71	0.00	0.00	0.00	0.71	0.29
Н	9	0.71	0.00	0.00	0.00	0.71	0.29
Н	10	0.71	0.00	0.00	0.00	0.71	0.29
С	1	1.26	3.01	0.00	0.00	4.27	-0.27
С	2	1.26	3.01	0.00	0.00	4.27	-0.27
Ĉ	3	1.26	3.03	0.00	0.00	1.28	0.28
c	3	1.20	2.00	0.00	0.00	4.26	0.26
		1.4.2	5.00	0.00	0.00	4.20	-0.20
Č				~ ~ ~	0.00	3 87	0.13
C	5	1.12	2.74	0.00		5.67	0.15
C C C	56	1.12 1.25	2.74 2.99	$\begin{array}{c} 0.00\\ 0.00\end{array}$	0.00	4.24	-0.24
C C C	5 6 7	1.12 1.25 1.26	2.74 2.99 3.02	$0.00 \\ 0.00 \\ 0.00$	0.00 0.00	4.24 4.27	-0.24 -0.27
C C C C	5 6 7 8	1.12 1.25 1.26 1.26	2.74 2.99 3.02 3.02	$0.00 \\ 0.00 \\ 0.00 \\ 0.00 \\ 0.00$	0.00 0.00 0.00	4.24 4.27 4.28	-0.24 -0.27 -0.28
	5 6 7 8 9	1.12 1.25 1.26 1.26 1.26	2.74 2.99 3.02 3.02 3.02	$\begin{array}{c} 0.00 \\ 0.00 \\ 0.00 \\ 0.00 \\ 0.00 \\ 0.00 \end{array}$	0.00 0.00 0.00 0.00	4.24 4.27 4.28 4.28	-0.24 -0.27 -0.28 -0.28
	5 6 7 8 9	1.12 1.25 1.26 1.26 1.26 1.26	2.74 2.99 3.02 3.02 3.03 2.98	$\begin{array}{c} 0.00 \\ 0.00 \\ 0.00 \\ 0.00 \\ 0.00 \\ 0.00 \\ 0.00 \end{array}$	0.00 0.00 0.00 0.00 0.00	4.24 4.27 4.28 4.28 4.25	-0.24 -0.27 -0.28 -0.28 -0.28
	5 6 7 8 9 10	1.12 1.25 1.26 1.26 1.26 1.27	2.74 2.99 3.02 3.02 3.03 2.98	$\begin{array}{c} 0.00\\$	0.00 0.00 0.00 0.00 0.00 0.00	4.24 4.27 4.28 4.28 4.25 2.88	-0.24 -0.27 -0.28 -0.28 -0.25
	5 6 7 8 9 10 11	1.12 1.25 1.26 1.26 1.26 1.27 1.13	2.74 2.99 3.02 3.02 3.03 2.98 2.75	$\begin{array}{c} 0.00\\ 0.00\\ 0.00\\ 0.00\\ 0.00\\ 0.00\\ 0.00\\ 0.00\\ 0.00\\ 0.00\\ \end{array}$	0.00 0.00 0.00 0.00 0.00 0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88	-0.24 -0.27 -0.28 -0.28 -0.25 0.12
	5 6 7 8 9 10 11 12	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25	2.74 2.99 3.02 3.02 3.03 2.98 2.75 3.02	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	4.24 4.27 4.28 4.28 4.25 3.88 4.27	-0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27
C C C C C C C C C C N	5 6 7 8 9 10 11 12 1	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85	-0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27 0.15
C C C C C C C C C C C C N N	5 6 7 8 9 10 11 12 1 2	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26	-0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26
C C C C C C C C C C C C C C N N O	5 6 7 8 9 10 11 12 1 2 1	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92	2.74 2.99 3.02 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48	-0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48
C C C C C C C C C N N O	5 6 7 8 9 10 11 12 1 2 1	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48	-0.24 -0.27 -0.28 -0.28 -0.25 -0.25 -0.25 -0.27 -0.27 -0.27 -0.26 -0.48
C C C C C C C C C C N N O	5 6 7 8 9 10 11 12 1 2 1 2	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.0	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48	-0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48
C C C C C C C C C C N N O	5 6 7 8 9 10 11 12 1 2 1 Atomic Populatio	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48	-0.24 -0.27 -0.28 -0.28 -0.25 -0.25 -0.27 -0.27 -0.27 -0.26 -0.48
C C C C C C C C C C C N N O Species	5 6 7 8 9 10 11 12 1 2 1 1 Atomic Populatio Ion	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ns (Mull s	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55	0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48	-0.24 -0.27 -0.28 -0.28 -0.25 -0.25 -0.12 -0.27 -0.15 -0.26 -0.48
C C C C C C C C C C C N N N O O Species	5 6 7 8 9 10 11 12 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.60	-0.24 -0.27 -0.28 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.30
C C C C C C C C C N N O O	5 6 7 8 9 10 11 12 1 2 1 2 1 2 1 2 1 2 1 2 1 2 1	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48	-0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.26 -0.48
C C C C C C C C C C C N N O Species H H H	5 6 7 8 9 10 11 12 1 2 1 1 Atomic Population 1 2 3	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 i ken) of p 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 AB d 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 <u>f</u> 0.00 0.00 0.00 0.00 0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.69 0.71	-0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 Charge(e) 0.30 0.31 0.29
C C C C C C C C C C C C N N O O Species H H H	5 6 7 8 9 10 11 12 1 2 1 1 Atomic Populatio 1 2 3 4	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71 0.71	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 AB d 0.00 0.0	0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.71	-0.24 -0.27 -0.28 -0.28 -0.28 -0.25 -0.12 -0.27 -0.27 -0.27 -0.26 -0.48 -0.48 -0.48 -0.30 -0.31 -0.29 -0.29
C C C C C C C C C C N N O Species H H H H H	5 6 7 8 9 10 11 12 1 2 1 Atomic Populatio 1 2 3 4 5	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71 0.71 0.71	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.75 <u>iken) of</u> 0.00 0.00 0.00 0.00 0.00	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48	-0.24 -0.27 -0.28 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.30 0.31 0.29 0.29 0.29
C C C C C C C C C C C N N O Species H H H H H H	5 6 7 8 9 10 11 12 1 2 1 1 Atomic Populatio 1 2 3 4 5 6	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00	0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.00 <u>f</u> <u>f</u> 0.00 0.	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48	-0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48
C C C C C C C C C C C C C C Species H H H H H H H H H H	5 6 7 8 9 10 11 12 1 2 1 1 Atomic Populatio 1 2 3 4 5 6 7	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.71 0.71 0.71 0.70 0.69	-0.24 -0.27 -0.28 -0.28 -0.25 -0.25 -0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.25 -0.26 -0.48 -0.29 -0.30 -0.31 -0.29 -0.29 -0.29 -0.29 -0.29 -0.30 -0.31
C C C C C C C C C C C C N N O O Species H H H H H H H H H H H H H H	5 6 7 8 9 10 11 12 1 2 1 Atomic Populatio 1 2 3 4 5 6 7 8	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71 0.71 0.71 0.70 0.69 0.71	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48	-0.24 -0.27 -0.28 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 Charge(e) 0.30 0.31 0.29 0.29 0.29 0.29 0.29 0.29 0.29 0.29
C C C C C C C C C C C C C Species H H H H H H H H H H H H H H H H H H H	5 6 7 8 9 10 11 12 1 2 1 1 2 1 1 2 1 1 2 1 2 1 1 2 3 4 5 6 7 8 8	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71 0.71 0.71 0.70 0.69 0.71 0.70 0.69 0.71 0.70 0.69 0.71 0.70 0.69 0.71 0.70 0.69 0.71 0.70 0.69 0.71 0.70 0.7	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total O.70 0.69 0.71 0.70 0.69 0.71 0.70 0.69 0.71 0.70 0.69 0.71	-0.24 -0.27 -0.28 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48
C C C C C C C C C C C C C C C Species H H H H H H H H H H H H H	5 6 7 8 9 10 11 12 1 2 1 1 Atomic Populatio 1 2 3 4 5 6 7 8 9	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull <u>s</u> 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71	-0.24 -0.27 -0.28 -0.28 -0.25 -0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.25 -0.26 -0.48 -0.29 -0.29 0.29 0.29 0.29 0.30 0.31 0.29 0.30 0.31 0.29 0.29 0.29 0.29
C C C C C C C C C C C C C C Species H H H H H H H H H H H H H H	5 6 7 8 9 10 11 12 1 2 1 1 2 1 1 2 1 1 2 1 1 2 3 4 5 6 7 8 9 9 10	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71 0.71 0.71 0.71 0.71	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71	-0.24 -0.27 -0.28 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.48 -0.48 -0.30 0.31 0.29 0.29 0.29 0.29 0.30 0.31 0.29 0.29 0.29 0.29 0.29 0.29 0.29 0.29
C C C C C C C C C C C C C C Species H H H H H H H H H H H H H H H C	5 6 7 8 9 10 11 12 1 2 1 1 2 1 1 2 1 1 2 3 4 5 6 7 8 9 10 1	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 0.70 0.69 0.71 0.71 0.71 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0.	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.69 0.71 0.71 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71	-0.24 -0.27 -0.28 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48
C C C C C C C C C C C C C C Species H H H H H H H H H H H H H H H H C C C	5 6 7 8 9 10 11 12 1 2 1 1 Atomic Populatio 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.72 0.28	-0.24 -0.27 -0.28 -0.28 -0.25 -0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.25 -0.48 -0.27 -0.26 -0.48 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.27 -0.28
C C C C C C C C C C C C C C Species H H H H H H H H H H H H H H H C C C C	5 6 7 8 9 10 11 12 1 2 1 1 2 1 1 2 1 1 2 1 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 1.13 1.58 1.92 1.071 0.71 0.71 1.26	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48	Charge(e) 0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 Charge(e) 0.30 0.31 0.29 0.28
C C C C C C C C C C C C C C C C C Species H H H H H H H H H H H H H C C C C C C	5 6 7 8 9 10 11 12 1 2 1 1 2 1 1 2 1 1 2 3 4 5 6 7 8 9 10 12 3 4 5 6 7 8 9 10	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total O.70 0.69 0.71 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.72 0.69 0.71 0.72 0.69 0.71 0.72 0.69 0.71 0.72 0.69 0.71 0.71 0.72 4.28 4.28 4.28 4.26	-0.24 -0.27 -0.28 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.48 -0.48 -0.25 -0.27 -0.27 -0.28 -0.29 0.29 0.29 0.29 0.29 0.29 0.29 0.29
C C C C C C C C C C C C C C C Species H H H H H H H H H H H H H H H C C C C	5 6 7 8 9 10 11 12 1 2 1 1 2 1 1 2 1 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 1 2 3 4 5 6 7 8 9 10	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 0.70 0.69 0.71 0.72 1.26 1.26 1.26 1.25 1.55 1	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of P 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.72 0.28 4.28 4.28 4.28 4.28 4.28 4.28 4.28 4.28	-0.24 -0.27 -0.28 -0.28 -0.25 -0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.25 -0.48 -0.27 -0.26 -0.48 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.27 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.29 -0.28 -0.28 -0.26 -0.28 -0.28 -0.27 -0.27 -0.27 -0.28 -0.28 -0.28 -0.27 -0.27 -0.27 -0.27 -0.28 -0.28 -0.28 -0.28 -0.26 -0.28 -0.29 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.29 -0.29 -0.27 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.26 -0.28 -0.28 -0.28 -0.26 -0.28 -0.26 -0.28 -0.26 -0.28 -0.26 -0.28 -0.26 -0.26 -0.28 -0.26 -0.25 -
C C C C C C C C C C C C C C Species H H H H H H H H H H H H H H H H H C	- 5 6 7 8 9 10 11 12 1 Atomic Population 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5	1.12 1.25 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 1.26 1.26 1.26 1.27 1.13 1.58 1.92 1.13 1.58 1.92 1.13 1.12 1.13 1.25 1.13 1.26 1.26 1.26 1.27 1.13 1.58 1.92 1.13 1.58 1.92 1.13 1.25 1.13 1.25 1.13 1.25 1.13 1.26 1.26 1.27 1.13 1.58 1.92 1.13 1.58 1.92 1.13 1.58 1.92 1.13 1.58 1.92 1.13 1.26 1.26 1.27 1.13 1.58 1.92 1.13 1.26 1.27 1.13 1.58 1.92 1.13 1.26 1.27 1.13 1.58 1.92 1.13 1.26 1.27 1.13 1.26 1.26 1.27 1.13 1.26 1.27 1.13 1.26 1.27 1.13 1.26 1.27 1.13 1.26 1.27 1.13 1.26 1.27 1.13 1.26 1.26 1.27 1.13 1.26 1.26 1.26 1.26 1.27 1.13 1.26 1.25 1.13	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of P 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48	Charge(e) 0.24 -0.27 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 Charge(e) 0.30 0.31 0.29 0.28 -0.28 -0.26 0.13 0.15 0.1
C C C C C C C C C C C C C N N O O Species H H H H H H H H H H H H H H H C C C C	5 6 7 8 9 10 11 12 1 2 1 1 2 1 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 6 7 8 9 9 10	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total O.70 0.69 0.71 0.70 0.69 0.71 0.72 0.69 0	-0.24 -0.27 -0.28 -0.28 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48
С С С С С С С С С С С С С С С С С С С	5 6 7 8 9 10 11 12 1 2 1 1 2 1 1 2 1 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.72 1.26 1.26 1.26 1.25 1.33 1.58 1.92 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.72 1.26 1.26 1.26 1.25 1.33 1.58 1.92 0.71 0.71 0.71 0.71 0.72 1.26 1.26 1.26 1.25 1.33 1.58 1.92 0.71 0.71 0.71 0.71 0.72 1.26 1.26 1.26 1.26 1.25 1.33 1.58 1.92 0.71 0.71 0.71 0.72 1.26 1.26 1.26 1.26 1.27 1.33 1.58 1.92 0.71 0.71 0.71 0.72 1.26	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of P 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.72 4.28 4.28 4.28 4.28 4.26 3.87 4.26 4.27	-0.24 -0.27 -0.28 -0.28 -0.25 -0.12 -0.27 0.15 -0.26 -0.48 -0.48 -0.25 -0.48 -0.27 -0.26 -0.48 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.28 -0.27 -0.28 -0.29 -0.28 -0.28 -0.28 -0.28 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.29 -0.28 -0.26 -0.28 -0.29 -0.27 -0.28 -0.26 -0.28 -0.26 -0.28 -0.26 -0.27 -0.28 -0.26 -0.26 -0.27 -0.28 -0.26 -0.26 -0.27 -0.28 -0.26 -0.27 -0.28 -0.26 -0.27 -0.26 -0.27 -0.26 -0.27 -0.26 -0.27 -0.27 -0.27 -0.26 -0.27 -0.27
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C C C C C C C C C C C C C C C C C C C	- 5 6 7 8 9 10 11 12 1 Atomic Population 1 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10	1.12 1.25 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71 0.72 0.26 1.26	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.72 4.28 4.2	-0.24 -0.27 -0.28 -0.28 -0.25 -0.25 -0.12 -0.27 0.15 -0.26 -0.48
C C C C C C C C C C C C C C C C C C C	- 5 6 7 8 9 10 11 12 1 2 1 Atomic Population 1 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 11 10 11 11	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 0.70 0.69 0.71 0.72 1.26 1	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total O.70 0.69 0.71 0.70 0.69 0.71 0.72 4.28 4.26 3.87 4.28 4.26 3.87 4	-0.24 -0.27 -0.28 -0.28 -0.25 -0.27 -0.27 0.15 -0.26 -0.48 -0.48 -0.48 -0.29 -0.29 0.29 0.29 0.29 0.29 0.29 0.29 0.29
C C C C C C C C C C C C C C C C C C C	5 6 7 8 9 10 11 12 1 2 1 1 Atomic Population 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 11 12 1 2 3 4 5 6 7 7 8 9 10 11 12 1 2 1 2 1 2 1 1 1 1 2 1 2 1 1 1 1 1 2 1 2 1 1 1 1 1 1 1 2 1 2 1 1 1 1 1 1 1 2 1	1.12 1.25 1.26 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 0.70 0.69 0.71 0.72 1.26 1	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of P 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.72 4.28 4.26 3.87 4.26 3.87 4.26	-0.24 -0.27 -0.28 -0.25 0.12 -0.27 0.15 -0.26 -0.48 Charge(e) 0.30 0.31 0.29 0.20 0.21 0.228 0.226 0.28 0.28 0.28 0.28 0.28 0.28 0.26 0.13
C C C C C C C C C C C C C C C C C C C	- 5 6 7 8 9 10 11 12 1 Atomic Populatio I 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 1 2 3 4 5 6 7 8 9 10 11 2 3 4 5 6 7 8 9 10 11 1 12 1	1.12 1.25 1.26 1.26 1.27 1.13 1.25 1.43 1.58 1.92 ms (Mull s 0.70 0.69 0.71 0.72 0.71 0.71 0.71 0.71 0.71 0.71 0.72 0.71 0.71 0.71 0.72 0.26 1.60	2.74 2.99 3.02 3.03 2.98 2.75 3.02 3.42 3.67 4.55 iken) of p 0.00 0.00 0.00 0.00 0.00 0.00 0.00 0	0.00 0.00	0.00 0.00	4.24 4.27 4.28 4.25 3.88 4.27 4.85 5.26 6.48 Total 0.70 0.69 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.71 0.72 4.28 4.28 4.28 4.28 4.28 4.26 3.87 4.26 3.87 4.26 3.87 4.26 3.87 4.26 3.87 4.26 5.25	-0.24 -0.27 -0.28 -0.28 -0.25 -0.12 -0.27 0.15 -0.26 -0.48 -0.26 -0.48 -0.29 0.29 0.29 0.29 0.29 0.29 0.29 0.29



Figure S19. ¹H NMR analysis of the crude products during different reaction time recorded in CDCl₃ for mechanistic study.



Figure S20. (a) Reusability of $HNT@B_{12}H_{12}@Au$ (conversions and selectivity are based on GC), (b) PXRD of recycled $HNT@B_{12}H_{12}@Au$ after seven cycles, (c) HRTEM of recycled $HNT@B_{12}H_{12}@Au$ after seven cycles, (d) HAADF-STEM image of $HNT@B_{12}H_{12}@Au$ after 7th use, and representative B, Au, Al, Si elemental mapping of (e), (f) XPS spectra of Au on the recycled $HNT@B_{12}H_{12}@Au$.



¹H NMR spectrum of (*E*)-1, 2-bisphenyldiazene recorded in CDCl₃, δ 7.99-7.97 (m, 4H), 7.58-7.50 (m, 6H).



¹³C NMR spectrum of (*E*)-1, 2-bisphenyldiazene recorded in CDCl₃, δ 152.68, 131.01, 129.11, 122.87.



¹H NMR spectrum of (E)-1, 2-bis (4-fluorophenyl)diazene recorded in CDCl₃, δ 7.81-7.77 (m, 4H), 7.15-7.11 (m, 4H).



 13 C NMR spectrum of (E)-1, 2-bis (4-fluorophenyl)diazene recorded in CDCl₃, δ 166.47(d, J = 337Hz), 146.76, 124.14(d, J = 9 Hz), 116.60(d, J = 23 Hz).



¹H NMR spectrum of (E)- 1, 2-bis(4-chlorophenyl)diazene recorded in CDCl₃, δ 7.75-7.73 (d, J=8 Hz, 4H), 7.44-7.41 (d, J=12 Hz, 4H).



¹³C NMR spectrum of (*E*)- 1, 2-bis(4-chlorophenyl)diazene recorded in CDCl₃, δ 148.85, 137.43, 129.74, 123.49.



¹H NMR spectrum of (E) -1,2-bis(4-bromophenyl)diazene recorded in CDCl₃, δ 7.73-7.71 (d, J=8 Hz, 4H), 7.59-7.57 (d, J=8 Hz, 4H).



¹³C NMR spectrum of (E) -1,2-bis(4-bromophenyl)diazene recorded in CDCl₃, δ 151.16, 132.43, 125.78, 124.44.



¹H NMR spectrum of (E) - 1,2-bis(4-iodophenyl) diazene recorded in CDCl₃, δ 7.88-7.86 (d, J=8 Hz, 4H), 7.60-7.58 (d, J=8 Hz, 4H).



¹³C NMR spectrum of (E) - 1,2-bis(4-iodophenyl) diazene recorded in CDCl₃, δ 152.86, 128.74, 123.81, 100.50.



¹H NMR spectrum of (E) - 1,2-bis(2-fluorophenyl) diazene recorded in CDCl₃, δ 7.95-7.92 (m, 2H), 7.89-7.86 (m, 2H), 7.45-7.40(m, 2H), 7.34-7.30(m, 2H).



 $\frac{13^{10}}{120} \frac{100}{190} \frac{1}{190} \frac{1}{100} \frac{1}{1$



¹H NMR spectrum of (E) -1,2-bis(3-bromophenyl)diazene recorded in CDCl₃, δ 7.98 (s, 2H), 7.82-7.80 (d, J=8 Hz, 2H), 7.56-7.54(d, J=8 Hz, 2H), 7.36-7.32(t, J=16 Hz, 2H).





¹H NMR spectrum of (E) -1,2-bis(3,4-dichlorophenyl)diazene recorded in CDCl₃, δ 8.02 (s, 2H), 7.81-7.78 (d, J=12 Hz, 2H), 7.63-7.61(d, J=8 Hz, 2H).





¹H NMR spectrum of (E) -1, 2-di-o-tolyldiazene recorded in CDCl₃, δ 7.73-7.71 (m, 2H), 7.28-7.27 (m, 4H), 7.19-7.17(m, 2H), 2.66(s, 6H).



 13 C NMR spectrum of (E) -1, 2-di-o-tolyldiazene recorded in CDCl₃, δ 153.42, 136.05, 131.43, 130.87, 126.92, 116.05, 18.15.



¹H NMR spectrum of (E) -1, 2-di-m-tolyldiazene recorded in CDCl₃, δ 7.66-7.64 (m, 4H), 7.35- 7.31(t, J=16 Hz, 2H), 7.22-7.20(d, J=8 Hz, 2H), 2.38(s, 6H).



¹³C NMR spectrum of (E) -1, 2-di-m-tolyldiazene recorded in CDCl₃, δ 152.80, 138.99, 131.71, 128.91, 122.87, 120.49, 21.39.



¹H NMR spectrum of (E) -1, 2-di-p-tolyldiazene recorded in CDCl₃, δ 7.69-7.67 (d, J=8 Hz, 4H), 7.24-7.22(d, J=8 Hz, 4H), 2.36(s, 6H).



¹³C NMR spectrum of (*E*) -1, 2-di-p-tolyldiazene recorded in CDCl₃, δ 152.78, 141.42, 129.99, 122.03, 21.50.



¹H NMR spectrum of (E) -1, 2-di-p-ethylphenyldiazene recorded in CDCl₃, δ 7.71-7.69 (d, J=8 Hz, 4H), 7.26-7.24(d, J=8 Hz, 4H), 2.66-2.59(m, 4H), 1.22-1.18(t, J=16 Hz, 6H).



¹³C NMR spectrum of (E) -1, 2-di-p-ethylphenyldiazene recorded in CDCl₃, δ 148.79, 147.70, 128.80, 122.13, 28.84, 14.99.



¹H NMR spectrum of (E) - 1, 2-bis(3,4-dimethylphenyl)diazene recorded in CDCl₃, δ 7.53-7.41 (d, J=8 Hz, 2H), 7.19(s, 2H), 6.81-6.79(d, J=8 Hz, 2H), 2.26(s, 6H), 2.15(s, 6H).



¹³C NMR spectrum of (E) - 1, 2-bis(3,4-dimethylphenyl)diazene recorded in CDCl₃, δ 148.78, 140.02, 135.52, 129.84, 122.65, 119.93, 20.70, 19.92.





¹³C NMR spectrum of (E) - 1, 2-bis(2, 3-dimethylphenyl)diazene recorded in CDCl₃, δ 151.10, 136.93, 132.48, 129.99, 125.12, 119.36, 21.86, 18.06.



¹H NMR spectrum of (E) - 1, 2-bis(3- chloro, 4-methylphenyl)diazene recorded in CDCl₃, δ 8.24-8.22 (d, J=8 Hz, 2H), 8.04(s, 2H), 7.42-7.40(d, J=8 Hz, 2H), 2.49(s, 6H).



 $\frac{1}{13}$ C NMR spectrum of (E) - 1, 2-bis(3- chloro, 4-methylphenyl)diazene recorded in CDCl₃, δ 152.10, 139.33, 135.47, 130.82, 124.27, 120.84, 20.26.



¹H NMR spectrum of (E) - 1, 2-bis(4-acetophenyl))diazene recorded in CDCl₃, δ 8.33-8.31 (d, J=8 Hz, 2H), 8.09-8.07(d, J=8 Hz, 2H), 2.44(s, 6H).





¹H NMR spectrum of (E) - 1, 2-bis(4-methoxylphenyl)diazene recorded in CDCl₃, δ 7.72-7.70 (d, J=8 Hz, 4H), 6.92-6.90(d, J=8 Hz, 2H), 3.78(s, 6H).



¹³C NMR spectrum of (E) - 1, 2-bis(4-methoxylphenyl)diazene recorded in CDCl₃, 161.85, 147.09, 123.37, 114.50, 55.65.



¹H NMR spectrum of (*E*) - 1, 2-bis(4-methoxylphenyl)diazene recorded in CDCl₃, δ 7.94-7.92 (d, *J*=8 Hz, 4H), 7.03-7.00(d, *J*=8 Hz, 4H), 4.17-4.12(m, 4H), 1.50-1.46(t, *J*=16 Hz, 6H).



¹³C NMR spectrum of (*E*) - 1, 2-bis(4-methoxylphenyl)diazene recorded in CDCl₃, δ 161.23, 146.48, 124.57, 114.73, 63.84, 14.78.



¹H NMR spectrum of (E) - 1, 2-bis (4-(trifluoromethyl) phenyl)diazene recorded in CDCl₃, δ 8.03-8.00 (d, J=8 Hz, 4H), 7.83-7.81(d, J=8 Hz, 4H).



210 200 190 150 170 160 150 140 130 120 110 100 90 50 70 60 50 f1 (ppm)

¹³C NMR spectrum of (*E*) - 1, 2-bis (4-(trifluoromethyl) phenyl)diazene recorded in CDCl₃, δ 152.19, 133.75-132.77 (q, *J*=32.7 Hz), 125.93-125.89(d, *J*=4.0 Hz), 125.73-122.28(d, *J*=345 Hz)121.873.



¹H NMR spectrum of (E) - -4, 4'-(diazene-1,2-diyl)dianiline recorded in CDCl₃, δ 7.68-7.65 (d, J=8 Hz, 4H), 6.67-6.65 (d, J=8 Hz, 4H), 3.88(s, 4H).



¹³C NMR spectrum of (E) - -4, 4'-(diazene-1,2-diyl)dianiline recorded in CDCl₃, δ 147.48, 144.79, 123.34, 113.76.



¹H NMR spectrum of (E) - 1, 2-bis (4-(methylthio)phenyl) diazene recorded in CDCl₃, δ 8.38-8.35 (d, J=8 Hz, 4H), 8.11-8.09(d, J=8 Hz, 4H), 3.05(s, 4H).



¹³C NMR spectrum of (E) - 1, 2-bis (4-(methylthio)phenyl) diazene recorded in CDCl₃, δ 143.75, 141.07, 125.35, 122.57, 15.22.



¹H NMR spectrum of (E) - 4,4'-(diazene-1,2-diyl)dibenzonitrile recorded in CDCl₃, δ 8.05-8.03 (d, J=8 Hz, 4H), 7.87-7.84(d, J=8 Hz, 4H).





¹H NMR spectrum of (*E*) - 1,2-bis([1,1'-biphenyl]-3-yl)diazene recorded in CDCl₃, δ 8.03 (s, 2H), 7.79-7.77(m, 2H), 7.66-7.60(m, 6H), 7.53-7.50(t,2H), 7.43-7.41(m,4H), 7.34-7.32(t, 2H).



¹³C NMR spectrum of (*E*) - 1,2-bis([1,1'-bipheny]]-3-yl)diazene recorded in CDCl₃, δ 150.48, 140.09, 138.69, 129.72, 129.41, 127.19, 126.93, 122.06, 121.16.

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