

## Yttrium and zirconium decorated $\text{Mg}_{12}\text{O}_{12}\text{-X}$ ( $\text{X} = \text{Y}, \text{Zr}$ ) nanoclusters as sensors for diazomethane ( $\text{CH}_2\text{N}_2$ ) gas

Terkumbur E. Gber <sup>a,b</sup>, Hitler Louis <sup>a,b,f\*\*</sup>, Obinna C. Ngana<sup>d</sup> Ismail O. Amodu <sup>a,c</sup>, Ernest E. Ekereke <sup>a,c</sup>, Innocent Benjamin <sup>a</sup>, Stephen A. Adalikwu<sup>a</sup> and Adedapo Adeyinka<sup>e</sup>

<sup>a</sup>Computational and Bio-Simulation Research Group, University of Calabar, Calabar, Nigeria

<sup>b</sup>Department of Pure and Applied Chemistry, Faculty of Physical Sciences, University of Calabar, Calabar, Nigeria

<sup>c</sup>Department of Mathematics, Faculty of Physical Sciences, University of Calabar, Calabar, Nigeria

<sup>d</sup>Department of Chemical Sciences, Federal University of Wukari, Wukari. Taraba State

<sup>e</sup>Department of Chemical Sciences, University of Johannesburg, South-Africa

<sup>f</sup>Faculty of Allied Health Sciences, Chettinad Hospital and Research institute, Chettinad Academy or Research and Education, Kelambakkam 603103, Tamil Nadu, India.

\*Corresponding authors' email: [louismuzong@gmail.com](mailto:louismuzong@gmail.com)

Electronic supporting information

**Table S1:** Optimized Parameters of the studied systems bond length and angles for the interacted systems. (Angstroms and Degrees)

### CH<sub>2</sub>N<sub>2</sub>@MgO

! Name	Definition	Value	Derivative Info.	!
! R1	R(1,13)	1.8896	-DE/DX = 0.0	!
! R2	R(1,15)	1.9487	-DE/DX = 0.0	!
! R3	R(1,16)	1.95	-DE/DX = 0.0	!
! R4	R(2,13)	1.9482	-DE/DX = 0.0	!
! R5	R(2,14)	1.8914	-DE/DX = 0.0	!
! R6	R(2,24)	1.9484	-DE/DX = 0.0	!
! R7	R(3,13)	1.9486	-DE/DX = 0.0	!

! R8	R(3,23)	1.8904	-DE/DX = 0.0	!
! R9	R(3,24)	1.9496	-DE/DX = 0.0	!
! R10	R(4,15)	1.8896	-DE/DX = 0.0	!
! R11	R(4,19)	1.9506	-DE/DX = 0.0	!
! R12	R(4,23)	1.9474	-DE/DX = 0.0	!
! R13	R(5,14)	1.9467	-DE/DX = 0.0	!
! R14	R(5,17)	1.9492	-DE/DX = 0.0	!
! R15	R(5,21)	1.8897	-DE/DX = 0.0	!
! R16	R(6,14)	1.9472	-DE/DX = 0.0	!
! R17	R(6,16)	1.8889	-DE/DX = 0.0	!
! R18	R(6,17)	1.9522	-DE/DX = 0.0	!
! R19	R(7,15)	1.946	-DE/DX = 0.0	!
! R20	R(7,16)	1.9477	-DE/DX = 0.0	!
! R21	R(7,18)	1.8923	-DE/DX = 0.0	!
! R22	R(8,18)	1.9431	-DE/DX = 0.0	!
! R23	R(8,19)	1.886	-DE/DX = 0.0	!
! R24	R(8,20)	1.981	-DE/DX = 0.0	!
! R25	R(9,17)	1.8864	-DE/DX = 0.0	!
! R26	R(9,18)	1.9413	-DE/DX = 0.0	!
! R27	R(9,20)	1.9608	-DE/DX = 0.0	!
! R28	R(10,20)	1.9063	-DE/DX = 0.0	!
! R29	R(10,21)	1.9436	-DE/DX = 0.0	!
! R30	R(10,22)	1.9397	-DE/DX = 0.0	!
! R31	R(11,19)	1.9486	-DE/DX = 0.0	!
! R32	R(11,22)	1.8906	-DE/DX = 0.0	!
! R33	R(11,23)	1.9491	-DE/DX = 0.0	!
! R34	R(12,21)	1.9513	-DE/DX = 0.0	!
! R35	R(12,22)	1.9482	-DE/DX = 0.0	!
! R36	R(12,24)	1.8883	-DE/DX = 0.0	!
! R37	R(13,14)	3.261	-DE/DX = 0.0	!

! R38	R(13,15)	3.2546	-DE/DX = 0.0	!
! R39	R(13,16)	3.255	-DE/DX = 0.0	!
! R40	R(13,23)	3.2607	-DE/DX = 0.0	!
! R41	R(13,24)	2.6835	-DE/DX = 0.0	!
! R42	R(14,16)	3.2569	-DE/DX = 0.0	!
! R43	R(14,17)	2.6862	-DE/DX = 0.0	!
! R44	R(14,21)	3.2576	-DE/DX = 0.0	!
! R45	R(14,24)	3.2553	-DE/DX = 0.0	!
! R46	R(15,16)	2.6835	-DE/DX = 0.0	!
! R47	R(15,18)	3.2547	-DE/DX = 0.0	!
! R48	R(15,19)	3.2546	-DE/DX = 0.0	!
! R49	R(15,23)	3.2601	-DE/DX = 0.0	!
! R50	R(16,17)	3.2589	-DE/DX = 0.0	!
! R51	R(16,18)	3.2537	-DE/DX = 0.0	!
! R52	R(17,18)	3.2393	-DE/DX = 0.0	!
! R53	R(17,20)	3.2945	-DE/DX = 0.0	!
! R54	R(17,21)	3.2344	-DE/DX = 0.0	!
! R55	R(18,19)	3.235	-DE/DX = 0.0	!
! R56	R(18,20)	2.702	-DE/DX = 0.0	!
! R57	R(19,20)	3.3004	-DE/DX = 0.0	!
! R58	R(19,22)	3.2278	-DE/DX = 0.0	!
! R59	R(19,23)	2.6846	-DE/DX = 0.0	!
! R60	R(20,21)	3.2954	-DE/DX = 0.0	!
! R61	R(20,22)	3.3041	-DE/DX = 0.0	!
! R62	R(20,25)	2.3306	-DE/DX = 0.0	!
! R63	R(21,22)	2.674	-DE/DX = 0.0	!
! R64	R(21,24)	3.2599	-DE/DX = 0.0	!
! R65	R(22,23)	3.2477	-DE/DX = 0.0	!
! R66	R(22,24)	3.2568	-DE/DX = 0.0	!
! R67	R(23,24)	3.2606	-DE/DX = 0.0	!

! R68	R(25,26)	1.1377	-DE/DX = 0.0	!
! R69	R(26,27)	1.277	-DE/DX = 0.0	!
! R70	R(27,28)	1.0786	-DE/DX = 0.0	!
! R71	R(27,29)	1.0787	-DE/DX = 0.0	!
! A1	A(1,13,2)	123.3916	-DE/DX = 0.0	!
! A2	A(1,13,3)	123.4384	-DE/DX = 0.0	!
! A3	A(1,13,14)	92.4504	-DE/DX = 0.0	!
! A4	A(1,13,23)	92.4901	-DE/DX = 0.0	!
! A5	A(1,13,24)	138.6372	-DE/DX = 0.0	!
! A6	A(2,13,3)	92.6892	-DE/DX = 0.0	!
! A7	A(2,13,15)	128.2018	-DE/DX = 0.0	!
! A8	A(2,13,16)	91.1994	-DE/DX = 0.0	!
! A9	A(2,13,23)	109.1956	-DE/DX = 0.0	!
! A10	A(3,13,14)	109.0672	-DE/DX = 0.0	!
! A11	A(3,13,15)	91.2633	-DE/DX = 0.0	!
! A12	A(3,13,16)	128.1405	-DE/DX = 0.0	!
! A13	A(14,13,15)	99.9811	-DE/DX = 0.0	!
! A14	A(14,13,23)	109.5299	-DE/DX = 0.0	!
! A15	A(15,13,24)	113.8432	-DE/DX = 0.0	!
! A16	A(16,13,23)	100.0193	-DE/DX = 0.0	!
! A17	A(16,13,24)	113.7357	-DE/DX = 0.0	!
! A18	A(2,14,5)	123.4432	-DE/DX = 0.0	!
! A19	A(2,14,6)	123.1852	-DE/DX = 0.0	!
! A20	A(2,14,16)	92.1899	-DE/DX = 0.0	!
! A21	A(2,14,17)	138.2759	-DE/DX = 0.0	!
! A22	A(2,14,21)	92.5398	-DE/DX = 0.0	!
! A23	A(5,14,6)	92.6587	-DE/DX = 0.0	!
! A24	A(5,14,13)	128.2051	-DE/DX = 0.0	!
! A25	A(5,14,16)	109.2089	-DE/DX = 0.0	!
! A26	A(5,14,24)	91.2602	-DE/DX = 0.0	!

! A27	A(6,14,13)	91.1699	-DE/DX = 0.0	!
! A28	A(6,14,21)	108.5817	-DE/DX = 0.0	!
! A29	A(6,14,24)	127.9809	-DE/DX = 0.0	!
! A30	A(13,14,17)	113.6515	-DE/DX = 0.0	!
! A31	A(13,14,21)	99.7935	-DE/DX = 0.0	!
! A32	A(16,14,21)	109.009	-DE/DX = 0.0	!
! A33	A(16,14,24)	99.8368	-DE/DX = 0.0	!
! A34	A(17,14,24)	113.5329	-DE/DX = 0.0	!
! A35	A(1,15,4)	123.398	-DE/DX = 0.0	!
! A36	A(1,15,7)	92.6806	-DE/DX = 0.0	!
! A37	A(1,15,18)	109.0686	-DE/DX = 0.0	!
! A38	A(1,15,19)	128.1302	-DE/DX = 0.0	!
! A39	A(1,15,23)	91.4097	-DE/DX = 0.0	!
! A40	A(4,15,7)	123.2286	-DE/DX = 0.0	!
! A41	A(4,15,13)	92.3206	-DE/DX = 0.0	!
! A42	A(4,15,16)	138.4523	-DE/DX = 0.0	!
! A43	A(4,15,18)	92.1178	-DE/DX = 0.0	!
! A44	A(7,15,13)	109.055	-DE/DX = 0.0	!
! A45	A(7,15,19)	90.9837	-DE/DX = 0.0	!
! A46	A(7,15,23)	128.0827	-DE/DX = 0.0	!
! A47	A(13,15,18)	109.188	-DE/DX = 0.0	!
! A48	A(13,15,19)	99.8448	-DE/DX = 0.0	!
! A49	A(16,15,19)	113.5711	-DE/DX = 0.0	!
! A50	A(16,15,23)	113.9056	-DE/DX = 0.0	!
! A51	A(18,15,23)	99.643	-DE/DX = 0.0	!
! A52	A(1,16,6)	123.5186	-DE/DX = 0.0	!
! A53	A(1,16,7)	92.5903	-DE/DX = 0.0	!
! A54	A(1,16,14)	91.4512	-DE/DX = 0.0	!
! A55	A(1,16,17)	128.2472	-DE/DX = 0.0	!
! A56	A(1,16,18)	109.0693	-DE/DX = 0.0	!

! A57	A(6,16,7)	123.2558	-DE/DX = 0.0	!
! A58	A(6,16,13)	92.4329	-DE/DX = 0.0	!
! A59	A(6,16,15)	138.5444	-DE/DX = 0.0	!
! A60	A(6,16,18)	92.0924	-DE/DX = 0.0	!
! A61	A(7,16,13)	108.9932	-DE/DX = 0.0	!
! A62	A(7,16,14)	128.1256	-DE/DX = 0.0	!
! A63	A(7,16,17)	91.0903	-DE/DX = 0.0	!
! A64	A(13,16,17)	99.9411	-DE/DX = 0.0	!
! A65	A(13,16,18)	109.2036	-DE/DX = 0.0	!
! A66	A(14,16,15)	113.9524	-DE/DX = 0.0	!
! A67	A(14,16,18)	99.6656	-DE/DX = 0.0	!
! A68	A(15,16,17)	113.7126	-DE/DX = 0.0	!
! A69	A(5,17,6)	92.4286	-DE/DX = 0.0	!
! A70	A(5,17,9)	123.9652	-DE/DX = 0.0	!
! A71	A(5,17,16)	109.062	-DE/DX = 0.0	!
! A72	A(5,17,18)	128.4124	-DE/DX = 0.0	!
! A73	A(5,17,20)	92.4467	-DE/DX = 0.0	!
! A74	A(6,17,9)	123.6015	-DE/DX = 0.0	!
! A75	A(6,17,18)	91.3548	-DE/DX = 0.0	!
! A76	A(6,17,20)	129.6596	-DE/DX = 0.0	!
! A77	A(6,17,21)	109.2961	-DE/DX = 0.0	!
! A78	A(9,17,14)	139.075	-DE/DX = 0.0	!
! A79	A(9,17,16)	92.6407	-DE/DX = 0.0	!
! A80	A(9,17,21)	92.3519	-DE/DX = 0.0	!
! A81	A(14,17,18)	113.8736	-DE/DX = 0.0	!
! A82	A(14,17,20)	115.5773	-DE/DX = 0.0	!
! A83	A(16,17,20)	101.1564	-DE/DX = 0.0	!
! A84	A(16,17,21)	109.532	-DE/DX = 0.0	!
! A85	A(18,17,21)	99.6325	-DE/DX = 0.0	!
! A86	A(7,18,8)	123.7929	-DE/DX = 0.0	!

! A87	A(7,18,9)	123.9125	-DE/DX = 0.0	!
! A88	A(7,18,17)	92.7198	-DE/DX = 0.0	!
! A89	A(7,18,19)	92.5812	-DE/DX = 0.0	!
! A90	A(7,18,20)	141.2734	-DE/DX = 0.0	!
! A91	A(8,18,9)	93.3912	-DE/DX = 0.0	!
! A92	A(8,18,15)	91.7932	-DE/DX = 0.0	!
! A93	A(8,18,16)	129.2676	-DE/DX = 0.0	!
! A94	A(8,18,17)	110.1134	-DE/DX = 0.0	!
! A95	A(9,18,15)	129.0101	-DE/DX = 0.0	!
! A96	A(9,18,16)	91.771	-DE/DX = 0.0	!
! A97	A(9,18,19)	109.6425	-DE/DX = 0.0	!
! A98	A(15,18,17)	100.2985	-DE/DX = 0.0	!
! A99	A(15,18,20)	116.2399	-DE/DX = 0.0	!
! A100	A(16,18,19)	100.1991	-DE/DX = 0.0	!
! A101	A(16,18,20)	116.1207	-DE/DX = 0.0	!
! A102	A(17,18,19)	109.7584	-DE/DX = 0.0	!
! A103	A(4,19,8)	123.8896	-DE/DX = 0.0	!
! A104	A(4,19,11)	92.5169	-DE/DX = 0.0	!
! A105	A(4,19,18)	91.5799	-DE/DX = 0.0	!
! A106	A(4,19,20)	129.8383	-DE/DX = 0.0	!
! A107	A(4,19,22)	109.2641	-DE/DX = 0.0	!
! A108	A(8,19,11)	124.7088	-DE/DX = 0.0	!
! A109	A(8,19,15)	92.872	-DE/DX = 0.0	!
! A110	A(8,19,22)	93.0191	-DE/DX = 0.0	!
! A111	A(8,19,23)	139.8312	-DE/DX = 0.0	!
! A112	A(11,19,15)	109.4707	-DE/DX = 0.0	!
! A113	A(11,19,18)	129.006	-DE/DX = 0.0	!
! A114	A(11,19,20)	92.7812	-DE/DX = 0.0	!
! A115	A(15,19,20)	101.233	-DE/DX = 0.0	!
! A116	A(15,19,22)	109.6408	-DE/DX = 0.0	!

! A117	A(18,19,22)	99.842	-DE/DX = 0.0	!
! A118	A(18,19,23)	114.1412	-DE/DX = 0.0	!
! A119	A(20,19,23)	115.6889	-DE/DX = 0.0	!
! A120	A(8,20,9)	91.6331	-DE/DX = 0.0	!
! A121	A(8,20,10)	119.9797	-DE/DX = 0.0	!
! A122	A(8,20,17)	107.0188	-DE/DX = 0.0	!
! A123	A(8,20,21)	124.5561	-DE/DX = 0.0	!
! A124	A(8,20,22)	89.0181	-DE/DX = 0.0	!
! A125	A(8,20,25)	92.4917	-DE/DX = 0.0	!
! A126	A(9,20,10)	120.5919	-DE/DX = 0.0	!
! A127	A(9,20,19)	106.6933	-DE/DX = 0.0	!
! A128	A(9,20,21)	89.1865	-DE/DX = 0.0	!
! A129	A(9,20,22)	124.3101	-DE/DX = 0.0	!
! A130	A(9,20,25)	123.341	-DE/DX = 0.0	!
! A131	A(10,20,17)	90.2452	-DE/DX = 0.0	!
! A132	A(10,20,18)	133.4066	-DE/DX = 0.0	!
! A133	A(10,20,19)	89.5639	-DE/DX = 0.0	!
! A134	A(10,20,25)	105.3679	-DE/DX = 0.0	!
! A135	A(17,20,19)	106.8321	-DE/DX = 0.0	!
! A136	A(17,20,22)	97.551	-DE/DX = 0.0	!
! A137	A(17,20,25)	144.694	-DE/DX = 0.0	!
! A138	A(18,20,21)	110.7205	-DE/DX = 0.0	!
! A139	A(18,20,22)	110.4401	-DE/DX = 0.0	!
! A140	A(18,20,25)	117.8927	-DE/DX = 0.0	!
! A141	A(19,20,21)	97.4424	-DE/DX = 0.0	!
! A142	A(19,20,25)	104.7882	-DE/DX = 0.0	!
! A143	A(21,20,25)	131.3418	-DE/DX = 0.0	!
! A144	A(22,20,25)	112.2455	-DE/DX = 0.0	!
! A145	A(5,21,10)	124.1639	-DE/DX = 0.0	!
! A146	A(5,21,12)	123.0293	-DE/DX = 0.0	!



! A147	A(5,21,20)	93.5482	-DE/DX = 0.0	!
! A148	A(5,21,22)	138.995	-DE/DX = 0.0	!
! A149	A(5,21,24)	92.1761	-DE/DX = 0.0	!
! A150	A(10,21,12)	92.7679	-DE/DX = 0.0	!
! A151	A(10,21,14)	128.3999	-DE/DX = 0.0	!
! A152	A(10,21,17)	91.3758	-DE/DX = 0.0	!
! A153	A(10,21,24)	109.1607	-DE/DX = 0.0	!
! A154	A(12,21,14)	91.1162	-DE/DX = 0.0	!
! A155	A(12,21,17)	128.3565	-DE/DX = 0.0	!
! A156	A(12,21,20)	110.3325	-DE/DX = 0.0	!
! A157	A(14,21,20)	101.3882	-DE/DX = 0.0	!
! A158	A(14,21,22)	113.8718	-DE/DX = 0.0	!
! A159	A(17,21,22)	113.941	-DE/DX = 0.0	!
! A160	A(17,21,24)	100.1253	-DE/DX = 0.0	!
! A161	A(20,21,24)	111.1851	-DE/DX = 0.0	!
! A162	A(10,22,11)	123.9906	-DE/DX = 0.0	!
! A163	A(10,22,12)	92.9842	-DE/DX = 0.0	!
! A164	A(10,22,19)	91.1431	-DE/DX = 0.0	!
! A165	A(10,22,23)	128.602	-DE/DX = 0.0	!
! A166	A(10,22,24)	109.3925	-DE/DX = 0.0	!
! A167	A(11,22,12)	123.6584	-DE/DX = 0.0	!
! A168	A(11,22,20)	93.7766	-DE/DX = 0.0	!
! A169	A(11,22,21)	139.5985	-DE/DX = 0.0	!
! A170	A(11,22,24)	92.7921	-DE/DX = 0.0	!
! A171	A(12,22,19)	128.5362	-DE/DX = 0.0	!
! A172	A(12,22,20)	110.094	-DE/DX = 0.0	!
! A173	A(12,22,23)	91.3892	-DE/DX = 0.0	!
! A174	A(19,22,21)	113.926	-DE/DX = 0.0	!
! A175	A(19,22,24)	100.2899	-DE/DX = 0.0	!
! A176	A(20,22,23)	101.6066	-DE/DX = 0.0	!

! A177	A(20,22,24)	111.0428	-DE/DX = 0.0	!
! A178	A(21,22,23)	114.2631	-DE/DX = 0.0	!
! A179	A(3,23,4)	123.1125	-DE/DX = 0.0	!
! A180	A(3,23,11)	123.6184	-DE/DX = 0.0	!
! A181	A(3,23,15)	92.1723	-DE/DX = 0.0	!
! A182	A(3,23,19)	137.9923	-DE/DX = 0.0	!
! A183	A(3,23,22)	92.3907	-DE/DX = 0.0	!
! A184	A(4,23,11)	92.6028	-DE/DX = 0.0	!
! A185	A(4,23,13)	91.0661	-DE/DX = 0.0	!
! A186	A(4,23,22)	108.6219	-DE/DX = 0.0	!
! A187	A(4,23,24)	127.8273	-DE/DX = 0.0	!
! A188	A(11,23,13)	128.5206	-DE/DX = 0.0	!
! A189	A(11,23,15)	109.2514	-DE/DX = 0.0	!
! A190	A(11,23,24)	91.5772	-DE/DX = 0.0	!
! A191	A(13,23,19)	113.4511	-DE/DX = 0.0	!
! A192	A(13,23,22)	99.79	-DE/DX = 0.0	!
! A193	A(15,23,22)	109.0112	-DE/DX = 0.0	!
! A194	A(15,23,24)	99.733	-DE/DX = 0.0	!
! A195	A(19,23,24)	113.3602	-DE/DX = 0.0	!
! A196	A(2,24,3)	92.651	-DE/DX = 0.0	!
! A197	A(2,24,12)	123.5045	-DE/DX = 0.0	!
! A198	A(2,24,21)	91.4061	-DE/DX = 0.0	!
! A199	A(2,24,22)	128.02	-DE/DX = 0.0	!
! A200	A(2,24,23)	109.1922	-DE/DX = 0.0	!
! A201	A(3,24,12)	123.0806	-DE/DX = 0.0	!
! A202	A(3,24,14)	109.2484	-DE/DX = 0.0	!
! A203	A(3,24,21)	127.8421	-DE/DX = 0.0	!
! A204	A(3,24,22)	91.0181	-DE/DX = 0.0	!
! A205	A(12,24,13)	138.3684	-DE/DX = 0.0	!
! A206	A(12,24,14)	92.3485	-DE/DX = 0.0	!

! A207	A(12,24,23)	92.1036	-DE/DX = 0.0	!
! A208	A(13,24,21)	113.6968	-DE/DX = 0.0	!
! A209	A(13,24,22)	113.5138	-DE/DX = 0.0	!
! A210	A(14,24,22)	99.7985	-DE/DX = 0.0	!
! A211	A(14,24,23)	109.6727	-DE/DX = 0.0	!
! A212	A(21,24,23)	99.6835	-DE/DX = 0.0	!
! A213	A(20,25,26)	115.1267	-DE/DX = 0.0	!
! A214	A(25,26,27)	179.3525	-DE/DX = 0.0	!
! A215	A(26,27,28)	117.8977	-DE/DX = 0.0	!
! A216	A(26,27,29)	117.3763	-DE/DX = 0.0	!
! A217	A(28,27,29)	124.7202	-DE/DX = 0.0	!

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**Table S2:** Optimized Parameters of the studied systems bond length and angles. (Angstroms and Degrees)

**CH2N2@YMgO**

! Name	Definition	Value	Derivative Info.	!
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! R1	R(1,13)	1.8847	-DE/DX = 0.0	!
! R2	R(1,15)	1.9353	-DE/DX = 0.0	!
! R3	R(1,16)	1.9475	-DE/DX = 0.0	!
! R4	R(2,13)	1.9477	-DE/DX = 0.0	!
! R5	R(2,14)	1.8915	-DE/DX = 0.0	!
! R6	R(2,24)	1.9452	-DE/DX = 0.0	!
! R7	R(3,13)	1.9443	-DE/DX = 0.0	!
! R8	R(3,23)	1.8779	-DE/DX = 0.0	!
! R9	R(3,24)	1.9514	-DE/DX = 0.0	!
! R10	R(4,15)	2.0084	-DE/DX = 0.0	!
! R11	R(4,19)	2.0474	-DE/DX = 0.0	!
! R12	R(4,25)	2.1401	-DE/DX = 0.0	!

! R13	R(5,14)	1.9496	-DE/DX = 0.0	!
! R14	R(5,17)	1.9484	-DE/DX = 0.0	!
! R15	R(5,21)	1.8884	-DE/DX = 0.0	!
! R16	R(6,14)	1.9475	-DE/DX = 0.0	!
! R17	R(6,16)	1.886	-DE/DX = 0.0	!
! R18	R(6,17)	1.9471	-DE/DX = 0.0	!
! R19	R(7,15)	1.9365	-DE/DX = 0.0	!
! R20	R(7,16)	1.9498	-DE/DX = 0.0	!
! R21	R(7,18)	1.8848	-DE/DX = 0.0	!
! R22	R(8,18)	1.9454	-DE/DX = 0.0	!
! R23	R(8,19)	1.8748	-DE/DX = 0.0	!
! R24	R(8,20)	1.954	-DE/DX = 0.0	!
! R25	R(9,17)	1.8922	-DE/DX = 0.0	!
! R26	R(9,18)	1.947	-DE/DX = 0.0	!
! R27	R(9,20)	1.9447	-DE/DX = 0.0	!
! R28	R(10,20)	1.8879	-DE/DX = 0.0	!
! R29	R(10,21)	1.9513	-DE/DX = 0.0	!
! R30	R(10,22)	1.9437	-DE/DX = 0.0	!
! R31	R(11,19)	1.922	-DE/DX = 0.0	!
! R32	R(11,22)	1.8957	-DE/DX = 0.0	!
! R33	R(11,23)	1.9287	-DE/DX = 0.0	!
! R34	R(12,21)	1.9492	-DE/DX = 0.0	!
! R35	R(12,22)	1.9422	-DE/DX = 0.0	!
! R36	R(12,24)	1.8882	-DE/DX = 0.0	!
! R37	R(13,14)	3.2706	-DE/DX = 0.0	!
! R38	R(13,15)	3.3169	-DE/DX = 0.0	!
! R39	R(13,16)	3.2492	-DE/DX = 0.0	!
! R40	R(13,23)	3.2994	-DE/DX = 0.0	!
! R41	R(13,24)	2.6847	-DE/DX = 0.0	!
! R42	R(14,16)	3.2473	-DE/DX = 0.0	!

! R43	R(14,17)	2.6894	-DE/DX = 0.0	!
! R44	R(14,21)	3.2616	-DE/DX = 0.0	!
! R45	R(14,24)	3.2485	-DE/DX = 0.0	!
! R46	R(15,16)	2.6921	-DE/DX = 0.0	!
! R47	R(15,18)	3.3285	-DE/DX = 0.0	!
! R48	R(15,19)	3.3746	-DE/DX = 0.0	!
! R49	R(15,25)	3.3945	-DE/DX = 0.0	!
! R50	R(16,17)	3.2514	-DE/DX = 0.0	!
! R51	R(16,18)	3.247	-DE/DX = 0.0	!
! R52	R(17,18)	3.2699	-DE/DX = 0.0	!
! R53	R(17,20)	3.2462	-DE/DX = 0.0	!
! R54	R(17,21)	3.2626	-DE/DX = 0.0	!
! R55	R(18,19)	3.2843	-DE/DX = 0.0	!
! R56	R(18,20)	2.6869	-DE/DX = 0.0	!
! R57	R(19,20)	3.2661	-DE/DX = 0.0	!
! R58	R(19,22)	3.2593	-DE/DX = 0.0	!
! R59	R(19,23)	2.7823	-DE/DX = 0.0	!
! R60	R(19,25)	3.6241	-DE/DX = 0.0	!
! R61	R(20,21)	3.2639	-DE/DX = 0.0	!
! R62	R(20,22)	3.2552	-DE/DX = 0.0	!
! R63	R(21,22)	2.6802	-DE/DX = 0.0	!
! R64	R(21,24)	3.2594	-DE/DX = 0.0	!
! R65	R(22,23)	3.2822	-DE/DX = 0.0	!
! R66	R(22,24)	3.2417	-DE/DX = 0.0	!
! R67	R(23,24)	3.2857	-DE/DX = 0.0	!
! R68	R(23,25)	3.5589	-DE/DX = 0.0	!
! R69	R(25,26)	2.1662	-DE/DX = 0.0	!
! R70	R(26,27)	1.232	-DE/DX = 0.0	!
! R71	R(27,28)	1.2842	-DE/DX = 0.0	!
! R72	R(28,29)	1.0895	-DE/DX = 0.0	!

! R73	R(28,30)	1.0811	-DE/DX = 0.0	!
! A1	A(1,13,2)	123.0884	-DE/DX = 0.0	!
! A2	A(1,13,3)	121.4562	-DE/DX = 0.0	!
! A3	A(1,13,14)	92.2844	-DE/DX = 0.0	!
! A4	A(1,13,23)	91.8508	-DE/DX = 0.0	!
! A5	A(1,13,24)	137.0821	-DE/DX = 0.0	!
! A6	A(2,13,3)	92.6907	-DE/DX = 0.0	!
! A7	A(2,13,15)	128.8616	-DE/DX = 0.0	!
! A8	A(2,13,16)	90.7244	-DE/DX = 0.0	!
! A9	A(2,13,23)	109.3423	-DE/DX = 0.0	!
! A10	A(3,13,14)	108.4779	-DE/DX = 0.0	!
! A11	A(3,13,15)	91.4129	-DE/DX = 0.0	!
! A12	A(3,13,16)	126.4839	-DE/DX = 0.0	!
! A13	A(14,13,15)	100.6148	-DE/DX = 0.0	!
! A14	A(14,13,23)	110.1909	-DE/DX = 0.0	!
! A15	A(15,13,23)	61.7164	-DE/DX = 0.0	!
! A16	A(15,13,24)	115.0595	-DE/DX = 0.0	!
! A17	A(16,13,23)	100.4656	-DE/DX = 0.0	!
! A18	A(16,13,24)	112.8387	-DE/DX = 0.0	!
! A19	A(2,14,5)	123.5497	-DE/DX = 0.0	!
! A20	A(2,14,6)	122.9388	-DE/DX = 0.0	!
! A21	A(2,14,16)	91.8116	-DE/DX = 0.0	!
! A22	A(2,14,17)	138.5466	-DE/DX = 0.0	!
! A23	A(2,14,21)	92.6271	-DE/DX = 0.0	!
! A24	A(5,14,6)	92.4306	-DE/DX = 0.0	!
! A25	A(5,14,13)	128.2288	-DE/DX = 0.0	!
! A26	A(5,14,16)	108.7427	-DE/DX = 0.0	!
! A27	A(5,14,24)	91.2412	-DE/DX = 0.0	!
! A28	A(6,14,13)	91.1859	-DE/DX = 0.0	!
! A29	A(6,14,21)	108.872	-DE/DX = 0.0	!

! A30	A(6,14,24)	127.7885	-DE/DX = 0.0	!
! A31	A(13,14,17)	114.0959	-DE/DX = 0.0	!
! A32	A(13,14,21)	100.1916	-DE/DX = 0.0	!
! A33	A(16,14,21)	109.0749	-DE/DX = 0.0	!
! A34	A(16,14,24)	99.3807	-DE/DX = 0.0	!
! A35	A(17,14,24)	113.8631	-DE/DX = 0.0	!
! A36	A(1,15,4)	122.1174	-DE/DX = 0.0	!
! A37	A(1,15,7)	92.6098	-DE/DX = 0.0	!
! A38	A(1,15,18)	106.8259	-DE/DX = 0.0	!
! A39	A(1,15,19)	123.6603	-DE/DX = 0.0	!
! A40	A(1,15,25)	132.6792	-DE/DX = 0.0	!
! A41	A(4,15,7)	121.0581	-DE/DX = 0.0	!
! A42	A(4,15,13)	93.0658	-DE/DX = 0.0	!
! A43	A(4,15,16)	137.7429	-DE/DX = 0.0	!
! A44	A(4,15,18)	92.3893	-DE/DX = 0.0	!
! A45	A(7,15,13)	107.0442	-DE/DX = 0.0	!
! A46	A(7,15,19)	87.6283	-DE/DX = 0.0	!
! A47	A(7,15,25)	134.3991	-DE/DX = 0.0	!
! A48	A(13,15,18)	107.2965	-DE/DX = 0.0	!
! A49	A(13,15,19)	97.9889	-DE/DX = 0.0	!
! A50	A(13,15,25)	111.9631	-DE/DX = 0.0	!
! A51	A(16,15,19)	110.4021	-DE/DX = 0.0	!
! A52	A(16,15,25)	174.0404	-DE/DX = 0.0	!
! A53	A(18,15,25)	113.7728	-DE/DX = 0.0	!
! A54	A(1,16,6)	124.1183	-DE/DX = 0.0	!
! A55	A(1,16,7)	91.8286	-DE/DX = 0.0	!
! A56	A(1,16,14)	91.8245	-DE/DX = 0.0	!
! A57	A(1,16,17)	128.8647	-DE/DX = 0.0	!
! A58	A(1,16,18)	109.4798	-DE/DX = 0.0	!
! A59	A(6,16,7)	124.0683	-DE/DX = 0.0	!

! A60	A(6,16,13)	92.9885	-DE/DX = 0.0	!
! A61	A(6,16,15)	142.134	-DE/DX = 0.0	!
! A62	A(6,16,18)	92.8058	-DE/DX = 0.0	!
! A63	A(7,16,13)	109.1578	-DE/DX = 0.0	!
! A64	A(7,16,14)	128.7994	-DE/DX = 0.0	!
! A65	A(7,16,17)	91.9043	-DE/DX = 0.0	!
! A66	A(13,16,17)	100.8643	-DE/DX = 0.0	!
! A67	A(13,16,18)	110.9508	-DE/DX = 0.0	!
! A68	A(14,16,15)	116.8704	-DE/DX = 0.0	!
! A69	A(14,16,18)	100.8704	-DE/DX = 0.0	!
! A70	A(15,16,17)	116.9921	-DE/DX = 0.0	!
! A71	A(5,17,6)	92.4796	-DE/DX = 0.0	!
! A72	A(5,17,9)	123.6819	-DE/DX = 0.0	!
! A73	A(5,17,16)	108.623	-DE/DX = 0.0	!
! A74	A(5,17,18)	128.2586	-DE/DX = 0.0	!
! A75	A(5,17,20)	91.2984	-DE/DX = 0.0	!
! A76	A(6,17,9)	122.7255	-DE/DX = 0.0	!
! A77	A(6,17,18)	90.9736	-DE/DX = 0.0	!
! A78	A(6,17,20)	127.7074	-DE/DX = 0.0	!
! A79	A(6,17,21)	108.8465	-DE/DX = 0.0	!
! A80	A(9,17,14)	138.4946	-DE/DX = 0.0	!
! A81	A(9,17,16)	91.7431	-DE/DX = 0.0	!
! A82	A(9,17,21)	92.7999	-DE/DX = 0.0	!
! A83	A(14,17,18)	113.9518	-DE/DX = 0.0	!
! A84	A(14,17,20)	113.8694	-DE/DX = 0.0	!
! A85	A(16,17,20)	99.3439	-DE/DX = 0.0	!
! A86	A(16,17,21)	108.9478	-DE/DX = 0.0	!
! A87	A(18,17,21)	100.2878	-DE/DX = 0.0	!
! A88	A(7,18,8)	121.0631	-DE/DX = 0.0	!
! A89	A(7,18,9)	123.4211	-DE/DX = 0.0	!



! A90	A(7,18,17)	92.5581	-DE/DX = 0.0	!
! A91	A(7,18,19)	91.1946	-DE/DX = 0.0	!
! A92	A(7,18,20)	136.9011	-DE/DX = 0.0	!
! A93	A(8,18,9)	92.6534	-DE/DX = 0.0	!
! A94	A(8,18,15)	91.3561	-DE/DX = 0.0	!
! A95	A(8,18,16)	126.4897	-DE/DX = 0.0	!
! A96	A(8,18,17)	108.4731	-DE/DX = 0.0	!
! A97	A(9,18,15)	128.8253	-DE/DX = 0.0	!
! A98	A(9,18,16)	90.8729	-DE/DX = 0.0	!
! A99	A(9,18,19)	108.8885	-DE/DX = 0.0	!
! A100	A(15,18,17)	100.5737	-DE/DX = 0.0	!
! A101	A(15,18,20)	114.915	-DE/DX = 0.0	!
! A102	A(16,18,19)	99.8269	-DE/DX = 0.0	!
! A103	A(16,18,20)	112.8461	-DE/DX = 0.0	!
! A104	A(17,18,19)	109.4734	-DE/DX = 0.0	!
! A105	A(4,19,8)	123.7437	-DE/DX = 0.0	!
! A106	A(4,19,11)	91.4215	-DE/DX = 0.0	!
! A107	A(4,19,18)	92.9466	-DE/DX = 0.0	!
! A108	A(4,19,20)	130.8012	-DE/DX = 0.0	!
! A109	A(4,19,22)	110.7715	-DE/DX = 0.0	!
! A110	A(4,19,23)	47.927	-DE/DX = 0.0	!
! A111	A(8,19,11)	123.1188	-DE/DX = 0.0	!
! A112	A(8,19,15)	91.209	-DE/DX = 0.0	!
! A113	A(8,19,22)	92.0061	-DE/DX = 0.0	!
! A114	A(8,19,23)	137.5805	-DE/DX = 0.0	!
! A115	A(8,19,25)	132.2704	-DE/DX = 0.0	!
! A116	A(11,19,15)	106.3066	-DE/DX = 0.0	!
! A117	A(11,19,18)	125.9372	-DE/DX = 0.0	!
! A118	A(11,19,20)	90.9839	-DE/DX = 0.0	!
! A119	A(11,19,25)	101.4767	-DE/DX = 0.0	!

! A120	A(15,19,20)	99.8681	-DE/DX = 0.0	!
! A121	A(15,19,22)	108.9975	-DE/DX = 0.0	!
! A122	A(15,19,23)	66.0845	-DE/DX = 0.0	!
! A123	A(18,19,22)	99.2888	-DE/DX = 0.0	!
! A124	A(18,19,23)	113.9672	-DE/DX = 0.0	!
! A125	A(18,19,25)	109.0995	-DE/DX = 0.0	!
! A126	A(20,19,23)	113.8199	-DE/DX = 0.0	!
! A127	A(20,19,25)	156.7149	-DE/DX = 0.0	!
! A128	A(22,19,25)	130.1673	-DE/DX = 0.0	!
! A129	A(8,20,9)	92.4599	-DE/DX = 0.0	!
! A130	A(8,20,10)	122.6357	-DE/DX = 0.0	!
! A131	A(8,20,17)	109.1032	-DE/DX = 0.0	!
! A132	A(8,20,21)	127.8444	-DE/DX = 0.0	!
! A133	A(8,20,22)	90.682	-DE/DX = 0.0	!
! A134	A(9,20,10)	123.8339	-DE/DX = 0.0	!
! A135	A(9,20,19)	109.6335	-DE/DX = 0.0	!
! A136	A(9,20,21)	91.7759	-DE/DX = 0.0	!
! A137	A(9,20,22)	128.0822	-DE/DX = 0.0	!
! A138	A(10,20,17)	92.4257	-DE/DX = 0.0	!
! A139	A(10,20,18)	138.7304	-DE/DX = 0.0	!
! A140	A(10,20,19)	92.1224	-DE/DX = 0.0	!
! A141	A(17,20,19)	110.5211	-DE/DX = 0.0	!
! A142	A(17,20,22)	99.7366	-DE/DX = 0.0	!
! A143	A(18,20,21)	114.505	-DE/DX = 0.0	!
! A144	A(18,20,22)	113.7662	-DE/DX = 0.0	!
! A145	A(19,20,21)	100.5977	-DE/DX = 0.0	!
! A146	A(5,21,10)	122.7717	-DE/DX = 0.0	!
! A147	A(5,21,12)	123.0035	-DE/DX = 0.0	!
! A148	A(5,21,20)	91.8694	-DE/DX = 0.0	!
! A149	A(5,21,22)	137.5102	-DE/DX = 0.0	!

! A150	A(5,21,24)	92.0413	-DE/DX = 0.0	!
! A151	A(10,21,12)	92.4683	-DE/DX = 0.0	!
! A152	A(10,21,14)	127.4341	-DE/DX = 0.0	!
! A153	A(10,21,17)	90.7607	-DE/DX = 0.0	!
! A154	A(10,21,24)	108.6489	-DE/DX = 0.0	!
! A155	A(12,21,14)	90.9448	-DE/DX = 0.0	!
! A156	A(12,21,17)	127.7825	-DE/DX = 0.0	!
! A157	A(12,21,20)	108.9555	-DE/DX = 0.0	!
! A158	A(14,21,20)	99.5856	-DE/DX = 0.0	!
! A159	A(14,21,22)	113.0621	-DE/DX = 0.0	!
! A160	A(17,21,22)	113.168	-DE/DX = 0.0	!
! A161	A(17,21,24)	99.7071	-DE/DX = 0.0	!
! A162	A(20,21,24)	109.1954	-DE/DX = 0.0	!
! A163	A(10,22,11)	122.8096	-DE/DX = 0.0	!
! A164	A(10,22,12)	92.9159	-DE/DX = 0.0	!
! A165	A(10,22,19)	91.3001	-DE/DX = 0.0	!
! A166	A(10,22,23)	130.2583	-DE/DX = 0.0	!
! A167	A(10,22,24)	109.5282	-DE/DX = 0.0	!
! A168	A(11,22,12)	123.0186	-DE/DX = 0.0	!
! A169	A(11,22,20)	91.7988	-DE/DX = 0.0	!
! A170	A(11,22,21)	137.8285	-DE/DX = 0.0	!
! A171	A(11,22,24)	91.6572	-DE/DX = 0.0	!
! A172	A(12,22,19)	130.0189	-DE/DX = 0.0	!
! A173	A(12,22,20)	109.4804	-DE/DX = 0.0	!
! A174	A(12,22,23)	91.919	-DE/DX = 0.0	!
! A175	A(19,22,21)	115.1869	-DE/DX = 0.0	!
! A176	A(19,22,24)	101.376	-DE/DX = 0.0	!
! A177	A(20,22,23)	101.8275	-DE/DX = 0.0	!
! A178	A(20,22,24)	109.8544	-DE/DX = 0.0	!
! A179	A(21,22,23)	115.8187	-DE/DX = 0.0	!

! A180	A(3,23,11)	121.2977	-DE/DX = 0.0	!
! A181	A(3,23,19)	134.6014	-DE/DX = 0.0	!
! A182	A(3,23,22)	90.7117	-DE/DX = 0.0	!
! A183	A(3,23,25)	131.3984	-DE/DX = 0.0	!
! A184	A(11,23,13)	124.1462	-DE/DX = 0.0	!
! A185	A(11,23,24)	89.7382	-DE/DX = 0.0	!
! A186	A(11,23,25)	103.5407	-DE/DX = 0.0	!
! A187	A(13,23,19)	111.9867	-DE/DX = 0.0	!
! A188	A(13,23,22)	98.2256	-DE/DX = 0.0	!
! A189	A(13,23,25)	108.3515	-DE/DX = 0.0	!
! A190	A(19,23,24)	111.7094	-DE/DX = 0.0	!
! A191	A(22,23,25)	131.751	-DE/DX = 0.0	!
! A192	A(24,23,25)	155.8379	-DE/DX = 0.0	!
! A193	A(2,24,3)	92.5514	-DE/DX = 0.0	!
! A194	A(2,24,12)	123.7581	-DE/DX = 0.0	!
! A195	A(2,24,21)	91.6886	-DE/DX = 0.0	!
! A196	A(2,24,22)	128.1615	-DE/DX = 0.0	!
! A197	A(2,24,23)	109.9317	-DE/DX = 0.0	!
! A198	A(3,24,12)	122.9063	-DE/DX = 0.0	!
! A199	A(3,24,14)	109.0924	-DE/DX = 0.0	!
! A200	A(3,24,21)	127.8749	-DE/DX = 0.0	!
! A201	A(3,24,22)	90.6162	-DE/DX = 0.0	!
! A202	A(12,24,13)	139.0791	-DE/DX = 0.0	!
! A203	A(12,24,14)	92.4692	-DE/DX = 0.0	!
! A204	A(12,24,23)	92.8237	-DE/DX = 0.0	!
! A205	A(13,24,21)	114.5727	-DE/DX = 0.0	!
! A206	A(13,24,22)	113.8608	-DE/DX = 0.0	!
! A207	A(14,24,22)	99.8646	-DE/DX = 0.0	!
! A208	A(14,24,23)	111.0953	-DE/DX = 0.0	!
! A209	A(21,24,23)	101.3058	-DE/DX = 0.0	!

! A210	A(4,25,23)	31.7948	-DE/DX = 0.0	!
! A211	A(15,25,23)	58.3678	-DE/DX = 0.0	!
! A212	A(15,25,26)	142.9217	-DE/DX = 0.0	!
! A213	A(19,25,26)	121.712	-DE/DX = 0.0	!
! A214	A(23,25,26)	152.2003	-DE/DX = 0.0	!
! A215	A(25,26,27)	179.7052	-DE/DX = 0.0	!
! A216	A(26,27,28)	137.2785	-DE/DX = 0.0	!
! A217	A(27,28,29)	120.7525	-DE/DX = 0.0	!
! A218	A(27,28,30)	118.274	-DE/DX = 0.0	!
! A219	A(29,28,30)	120.9734	-DE/DX = 0.0	!
! A220	L(4,25,26,23,-1)	183.9952	-DE/DX = 0.0	!
! A221	L(4,25,26,23,-2)	243.6788	-DE/DX = 0.0	!

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**Table S3:** Optimized Parameters of the studied systems bond length and angles for the interacted systems. (Angstroms and Degrees)

**CH2N2@ZrMgO**

Name	Definition	Value	Derivative Info.	!
-----				
! R1	R(1,13)	1.8898	-DE/DX = 0.0	!
! R2	R(1,15)	1.9356	-DE/DX = 0.0	!
! R3	R(1,16)	1.9493	-DE/DX = 0.0	!
! R4	R(2,13)	1.9501	-DE/DX = 0.0	!
! R5	R(2,14)	1.8925	-DE/DX = 0.0	!
! R6	R(2,24)	1.9451	-DE/DX = 0.0	!
! R7	R(3,13)	1.9463	-DE/DX = 0.0	!
! R8	R(3,23)	1.8849	-DE/DX = 0.0	!
! R9	R(3,24)	1.9427	-DE/DX = 0.0	!
! R10	R(4,19)	3.1197	-DE/DX = 0.0	!
! R11	R(4,23)	1.9897	-DE/DX = 0.0	!
! R12	R(4,25)	1.9611	-DE/DX = 0.0	!

! R13	R(5,14)	1.95	-DE/DX = 0.0	!
! R14	R(5,17)	1.9514	-DE/DX = 0.0	!
! R15	R(5,21)	1.8907	-DE/DX = 0.0	!
! R16	R(6,14)	1.9471	-DE/DX = 0.0	!
! R17	R(6,16)	1.885	-DE/DX = 0.0	!
! R18	R(6,17)	1.9456	-DE/DX = 0.0	!
! R19	R(7,15)	1.9272	-DE/DX = 0.0	!
! R20	R(7,16)	1.9519	-DE/DX = 0.0	!
! R21	R(7,18)	1.89	-DE/DX = 0.0	!
! R22	R(8,18)	1.9366	-DE/DX = 0.0	!
! R23	R(8,19)	1.8874	-DE/DX = 0.0	!
! R24	R(8,20)	1.9383	-DE/DX = 0.0	!
! R25	R(9,17)	1.8863	-DE/DX = 0.0	!
! R26	R(9,18)	1.9573	-DE/DX = 0.0	!
! R27	R(9,20)	1.9398	-DE/DX = 0.0	!
! R28	R(10,20)	1.8892	-DE/DX = 0.0	!
! R29	R(10,21)	1.9498	-DE/DX = 0.0	!
! R30	R(10,22)	1.9453	-DE/DX = 0.0	!
! R31	R(11,19)	1.9343	-DE/DX = 0.0	!
! R32	R(11,22)	1.9017	-DE/DX = 0.0	!
! R33	R(11,23)	1.9179	-DE/DX = 0.0	!
! R34	R(12,21)	1.9497	-DE/DX = 0.0	!
! R35	R(12,22)	1.9406	-DE/DX = 0.0	!
! R36	R(12,24)	1.885	-DE/DX = 0.0	!
! R37	R(13,14)	3.2707	-DE/DX = 0.0	!
! R38	R(13,15)	3.2759	-DE/DX = 0.0	!
! R39	R(13,16)	3.2218	-DE/DX = 0.0	!
! R40	R(13,23)	3.2981	-DE/DX = 0.0	!
! R41	R(13,24)	2.6843	-DE/DX = 0.0	!
! R42	R(14,16)	3.2513	-DE/DX = 0.0	!

! R43	R(14,17)	2.6867	-DE/DX = 0.0	!
! R44	R(14,21)	3.2774	-DE/DX = 0.0	!
! R45	R(14,24)	3.2302	-DE/DX = 0.0	!
! R46	R(15,16)	2.6891	-DE/DX = 0.0	!
! R47	R(15,18)	3.3533	-DE/DX = 0.0	!
! R48	R(15,25)	3.4247	-DE/DX = 0.0	!
! R49	R(16,17)	3.2329	-DE/DX = 0.0	!
! R50	R(16,18)	3.2663	-DE/DX = 0.0	!
! R51	R(17,18)	3.2949	-DE/DX = 0.0	!
! R52	R(17,20)	3.255	-DE/DX = 0.0	!
! R53	R(17,21)	3.2546	-DE/DX = 0.0	!
! R54	R(18,19)	3.4431	-DE/DX = 0.0	!
! R55	R(18,20)	2.6688	-DE/DX = 0.0	!
! R56	R(19,20)	3.3114	-DE/DX = 0.0	!
! R57	R(19,22)	3.2693	-DE/DX = 0.0	!
! R58	R(19,23)	3.1388	-DE/DX = 0.0	!
! R59	R(20,21)	3.2613	-DE/DX = 0.0	!
! R60	R(20,22)	3.2067	-DE/DX = 0.0	!
! R61	R(21,22)	2.6765	-DE/DX = 0.0	!
! R62	R(21,24)	3.2679	-DE/DX = 0.0	!
! R63	R(22,23)	3.2203	-DE/DX = 0.0	!
! R64	R(22,24)	3.235	-DE/DX = 0.0	!
! R65	R(23,24)	3.2995	-DE/DX = 0.0	!
! R66	R(25,26)	1.892	-DE/DX = -0.0001	!
! R67	R(26,27)	1.3507	-DE/DX = 0.0	!
! R68	R(27,28)	1.2756	-DE/DX = 0.0001	!
! R69	R(28,29)	1.0887	-DE/DX = 0.0	!
! R70	R(28,30)	1.0835	-DE/DX = 0.0	!
! A1	A(19,4,25)	78.2847	-DE/DX = 0.0	!
! A2	A(23,4,25)	121.2565	-DE/DX = 0.0	!

! A3	A(1,13,2)	123.9468	-DE/DX = 0.0	!
! A4	A(1,13,3)	121.8891	-DE/DX = 0.0	!
! A5	A(1,13,14)	93.3107	-DE/DX = 0.0	!
! A6	A(1,13,23)	92.0345	-DE/DX = 0.0	!
! A7	A(1,13,24)	138.8787	-DE/DX = 0.0	!
! A8	A(2,13,3)	92.5143	-DE/DX = 0.0	!
! A9	A(2,13,15)	130.7584	-DE/DX = 0.0	!
! A10	A(2,13,16)	91.1425	-DE/DX = 0.0	!
! A11	A(2,13,23)	109.3943	-DE/DX = 0.0	!
! A12	A(3,13,14)	107.3302	-DE/DX = 0.0	!
! A13	A(3,13,15)	90.4673	-DE/DX = 0.0	!
! A14	A(3,13,16)	124.3507	-DE/DX = 0.0	!
! A15	A(14,13,15)	102.1996	-DE/DX = 0.0	!
! A16	A(14,13,23)	108.9818	-DE/DX = 0.0	!
! A17	A(15,13,23)	60.5332	-DE/DX = 0.0	!
! A18	A(15,13,24)	116.0143	-DE/DX = 0.0	!
! A19	A(16,13,23)	98.1214	-DE/DX = 0.0	!
! A20	A(16,13,24)	112.3412	-DE/DX = 0.0	!
! A21	A(2,14,5)	123.9138	-DE/DX = 0.0	!
! A22	A(2,14,6)	122.2208	-DE/DX = 0.0	!
! A23	A(2,14,16)	91.3075	-DE/DX = 0.0	!
! A24	A(2,14,17)	137.9954	-DE/DX = 0.0	!
! A25	A(2,14,21)	93.3296	-DE/DX = 0.0	!
! A26	A(5,14,6)	92.5502	-DE/DX = 0.0	!
! A27	A(5,14,13)	128.1725	-DE/DX = 0.0	!
! A28	A(5,14,16)	108.4849	-DE/DX = 0.0	!
! A29	A(5,14,24)	91.0925	-DE/DX = 0.0	!
! A30	A(6,14,13)	90.4085	-DE/DX = 0.0	!
! A31	A(6,14,21)	108.6319	-DE/DX = 0.0	!
! A32	A(6,14,24)	126.9758	-DE/DX = 0.0	!



! A33	A(13,14,17)	113.2007	-DE/DX = 0.0	!
! A34	A(13,14,21)	100.5734	-DE/DX = 0.0	!
! A35	A(16,14,21)	108.6694	-DE/DX = 0.0	!
! A36	A(16,14,24)	98.6373	-DE/DX = 0.0	!
! A37	A(17,14,24)	113.0139	-DE/DX = 0.0	!
! A38	A(1,15,7)	92.8883	-DE/DX = 0.0	!
! A39	A(1,15,18)	106.9549	-DE/DX = 0.0	!
! A40	A(1,15,25)	143.7495	-DE/DX = 0.0	!
! A41	A(7,15,13)	106.0693	-DE/DX = 0.0	!
! A42	A(7,15,25)	119.9297	-DE/DX = 0.0	!
! A43	A(13,15,18)	105.7023	-DE/DX = 0.0	!
! A44	A(13,15,25)	117.2741	-DE/DX = 0.0	!
! A45	A(18,15,25)	97.8449	-DE/DX = 0.0	!
! A46	A(1,16,6)	124.5714	-DE/DX = 0.0	!
! A47	A(1,16,7)	91.7097	-DE/DX = 0.0	!
! A48	A(1,16,14)	92.7679	-DE/DX = 0.0	!
! A49	A(1,16,17)	131.0	-DE/DX = 0.0	!
! A50	A(1,16,18)	109.7724	-DE/DX = 0.0	!
! A51	A(6,16,7)	124.8192	-DE/DX = 0.0	!
! A52	A(6,16,13)	93.05	-DE/DX = 0.0	!
! A53	A(6,16,15)	143.9918	-DE/DX = 0.0	!
! A54	A(6,16,18)	93.8705	-DE/DX = 0.0	!
! A55	A(7,16,13)	107.3506	-DE/DX = 0.0	!
! A56	A(7,16,14)	128.0145	-DE/DX = 0.0	!
! A57	A(7,16,17)	92.0413	-DE/DX = 0.0	!
! A58	A(13,16,17)	101.0918	-DE/DX = 0.0	!
! A59	A(13,16,18)	109.0588	-DE/DX = 0.0	!
! A60	A(14,16,15)	117.7979	-DE/DX = 0.0	!
! A61	A(14,16,18)	100.4733	-DE/DX = 0.0	!
! A62	A(15,16,17)	118.9981	-DE/DX = 0.0	!

! A63	A(5,17,6)	92.5509	-DE/DX = 0.0	!
! A64	A(5,17,9)	123.5936	-DE/DX = 0.0	!
! A65	A(5,17,16)	109.1267	-DE/DX = 0.0	!
! A66	A(5,17,18)	126.7283	-DE/DX = 0.0	!
! A67	A(5,17,20)	91.5309	-DE/DX = 0.0	!
! A68	A(6,17,9)	122.8619	-DE/DX = 0.0	!
! A69	A(6,17,18)	91.8393	-DE/DX = 0.0	!
! A70	A(6,17,20)	129.5811	-DE/DX = 0.0	!
! A71	A(6,17,21)	109.5239	-DE/DX = 0.0	!
! A72	A(9,17,14)	138.3207	-DE/DX = 0.0	!
! A73	A(9,17,16)	91.3928	-DE/DX = 0.0	!
! A74	A(9,17,21)	92.3219	-DE/DX = 0.0	!
! A75	A(14,17,18)	113.3833	-DE/DX = 0.0	!
! A76	A(14,17,20)	115.0876	-DE/DX = 0.0	!
! A77	A(16,17,20)	100.7238	-DE/DX = 0.0	!
! A78	A(16,17,21)	109.6919	-DE/DX = 0.0	!
! A79	A(18,17,21)	98.498	-DE/DX = 0.0	!
! A80	A(7,18,8)	127.8028	-DE/DX = 0.0	!
! A81	A(7,18,9)	121.0556	-DE/DX = 0.0	!
! A82	A(7,18,17)	91.3001	-DE/DX = 0.0	!
! A83	A(7,18,19)	102.3634	-DE/DX = 0.0	!
! A84	A(7,18,20)	139.7339	-DE/DX = 0.0	!
! A85	A(8,18,9)	92.575	-DE/DX = 0.0	!
! A86	A(8,18,15)	99.0863	-DE/DX = 0.0	!
! A87	A(8,18,16)	132.5276	-DE/DX = 0.0	!
! A88	A(8,18,17)	109.3108	-DE/DX = 0.0	!
! A89	A(9,18,15)	129.2561	-DE/DX = 0.0	!
! A90	A(9,18,16)	89.1331	-DE/DX = 0.0	!
! A91	A(9,18,19)	109.6527	-DE/DX = 0.0	!
! A92	A(15,18,17)	100.4595	-DE/DX = 0.0	!

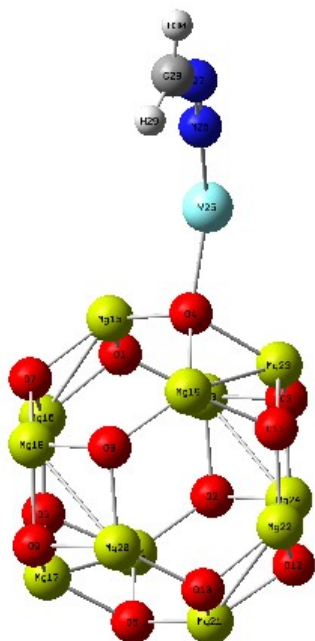
! A93	A(15,18,19)	73.6845	-DE/DX = 0.0	!
! A94	A(15,18,20)	120.2386	-DE/DX = 0.0	!
! A95	A(16,18,19)	112.121	-DE/DX = 0.0	!
! A96	A(16,18,20)	114.2897	-DE/DX = 0.0	!
! A97	A(17,18,19)	114.933	-DE/DX = 0.0	!
! A98	A(4,19,8)	105.9788	-DE/DX = 0.0	!
! A99	A(4,19,11)	72.3272	-DE/DX = 0.0	!
! A100	A(4,19,18)	79.8608	-DE/DX = 0.0	!
! A101	A(4,19,20)	113.4943	-DE/DX = 0.0	!
! A102	A(4,19,22)	94.5911	-DE/DX = 0.0	!
! A103	A(8,19,11)	114.3562	-DE/DX = 0.0	!
! A104	A(8,19,22)	87.6125	-DE/DX = 0.0	!
! A105	A(8,19,23)	114.8467	-DE/DX = 0.0	!
! A106	A(11,19,18)	107.6868	-DE/DX = 0.0	!
! A107	A(11,19,20)	87.8599	-DE/DX = 0.0	!
! A108	A(18,19,22)	90.9817	-DE/DX = 0.0	!
! A109	A(18,19,23)	94.4717	-DE/DX = 0.0	!
! A110	A(20,19,23)	102.1442	-DE/DX = 0.0	!
! A111	A(8,20,9)	93.0657	-DE/DX = 0.0	!
! A112	A(8,20,10)	121.5767	-DE/DX = 0.0	!
! A113	A(8,20,17)	110.7695	-DE/DX = 0.0	!
! A114	A(8,20,21)	128.166	-DE/DX = 0.0	!
! A115	A(8,20,22)	88.6003	-DE/DX = 0.0	!
! A116	A(9,20,10)	123.3936	-DE/DX = 0.0	!
! A117	A(9,20,19)	115.3013	-DE/DX = 0.0	!
! A118	A(9,20,21)	91.1287	-DE/DX = 0.0	!
! A119	A(9,20,22)	125.014	-DE/DX = 0.0	!
! A120	A(10,20,17)	92.2692	-DE/DX = 0.0	!
! A121	A(10,20,18)	136.2082	-DE/DX = 0.0	!
! A122	A(10,20,19)	92.1773	-DE/DX = 0.0	!

! A123	A(17,20,19)	119.8051	-DE/DX = 0.0	!
! A124	A(17,20,22)	98.5229	-DE/DX = 0.0	!
! A125	A(18,20,21)	113.2062	-DE/DX = 0.0	!
! A126	A(18,20,22)	108.8243	-DE/DX = 0.0	!
! A127	A(19,20,21)	105.6986	-DE/DX = 0.0	!
! A128	A(5,21,10)	123.4689	-DE/DX = 0.0	!
! A129	A(5,21,12)	121.7845	-DE/DX = 0.0	!
! A130	A(5,21,20)	92.4732	-DE/DX = 0.0	!
! A131	A(5,21,22)	135.4761	-DE/DX = 0.0	!
! A132	A(5,21,24)	91.0362	-DE/DX = 0.0	!
! A133	A(10,21,12)	92.3781	-DE/DX = 0.0	!
! A134	A(10,21,14)	128.3841	-DE/DX = 0.0	!
! A135	A(10,21,17)	91.1611	-DE/DX = 0.0	!
! A136	A(10,21,24)	109.2715	-DE/DX = 0.0	!
! A137	A(12,21,14)	90.0444	-DE/DX = 0.0	!
! A138	A(12,21,17)	125.9199	-DE/DX = 0.0	!
! A139	A(12,21,20)	108.3218	-DE/DX = 0.0	!
! A140	A(14,21,20)	100.3809	-DE/DX = 0.0	!
! A141	A(14,21,22)	111.6489	-DE/DX = 0.0	!
! A142	A(17,21,22)	110.9038	-DE/DX = 0.0	!
! A143	A(17,21,24)	98.563	-DE/DX = 0.0	!
! A144	A(20,21,24)	109.4591	-DE/DX = 0.0	!
! A145	A(10,22,11)	123.7017	-DE/DX = 0.0	!
! A146	A(10,22,12)	92.7959	-DE/DX = 0.0	!
! A147	A(10,22,19)	92.4203	-DE/DX = 0.0	!
! A148	A(10,22,23)	132.5609	-DE/DX = 0.0	!
! A149	A(10,22,24)	110.6427	-DE/DX = 0.0	!
! A150	A(11,22,12)	125.5627	-DE/DX = 0.0	!
! A151	A(11,22,20)	91.5466	-DE/DX = 0.0	!
! A152	A(11,22,21)	139.7736	-DE/DX = 0.0	!

! A153	A(11,22,24)	94.1632	-DE/DX = 0.0	!
! A154	A(12,22,19)	143.1036	-DE/DX = 0.0	!
! A155	A(12,22,20)	110.6339	-DE/DX = 0.0	!
! A156	A(12,22,23)	92.9929	-DE/DX = 0.0	!
! A157	A(19,22,21)	123.242	-DE/DX = 0.0	!
! A158	A(19,22,24)	113.7377	-DE/DX = 0.0	!
! A159	A(20,22,23)	102.6897	-DE/DX = 0.0	!
! A160	A(20,22,24)	111.6884	-DE/DX = 0.0	!
! A161	A(21,22,23)	116.9255	-DE/DX = 0.0	!
! A162	A(3,23,4)	115.9934	-DE/DX = 0.0	!
! A163	A(3,23,11)	122.7683	-DE/DX = 0.0	!
! A164	A(3,23,19)	142.3977	-DE/DX = 0.0	!
! A165	A(3,23,22)	90.4153	-DE/DX = 0.0	!
! A166	A(4,23,11)	106.5418	-DE/DX = 0.0	!
! A167	A(4,23,13)	87.5127	-DE/DX = 0.0	!
! A168	A(4,23,22)	127.0675	-DE/DX = 0.0	!
! A169	A(4,23,24)	132.2666	-DE/DX = 0.0	!
! A170	A(11,23,13)	126.6462	-DE/DX = 0.0	!
! A171	A(11,23,24)	91.8544	-DE/DX = 0.0	!
! A172	A(13,23,19)	123.4865	-DE/DX = 0.0	!
! A173	A(13,23,22)	98.859	-DE/DX = 0.0	!
! A174	A(19,23,24)	115.5377	-DE/DX = 0.0	!
! A175	A(2,24,3)	92.7838	-DE/DX = 0.0	!
! A176	A(2,24,12)	124.492	-DE/DX = 0.0	!
! A177	A(2,24,21)	92.6226	-DE/DX = 0.0	!
! A178	A(2,24,22)	128.2368	-DE/DX = 0.0	!
! A179	A(2,24,23)	109.4877	-DE/DX = 0.0	!
! A180	A(3,24,12)	121.3138	-DE/DX = 0.0	!
! A181	A(3,24,14)	108.9222	-DE/DX = 0.0	!
! A182	A(3,24,21)	126.849	-DE/DX = 0.0	!

! A183	A(3,24,22)	88.9621	-DE/DX = 0.0	!
! A184	A(12,24,13)	138.9992	-DE/DX = 0.0	!
! A185	A(12,24,14)	92.6601	-DE/DX = 0.0	!
! A186	A(12,24,23)	91.6076	-DE/DX = 0.0	!
! A187	A(13,24,21)	115.2698	-DE/DX = 0.0	!
! A188	A(13,24,22)	113.225	-DE/DX = 0.0	!
! A189	A(14,24,22)	99.5801	-DE/DX = 0.0	!
! A190	A(14,24,23)	109.9446	-DE/DX = 0.0	!
! A191	A(21,24,23)	100.0806	-DE/DX = 0.0	!
! A192	A(4,25,15)	29.0483	-DE/DX = 0.0	!
! A193	A(4,25,26)	108.793	-DE/DX = 0.0	!
! A194	A(15,25,26)	113.3599	-DE/DX = 0.0	!
! A195	A(25,26,27)	166.3746	-DE/DX = 0.0	!
! A196	A(26,27,28)	120.6198	-DE/DX = 0.0001	!
! A197	A(27,28,29)	120.794	-DE/DX = 0.0	!
! A198	A(27,28,30)	118.1379	-DE/DX = 0.0	!
! A199	A(29,28,30)	121.068	-DE/DX = 0.0	!
! A200	L(16,15,25,3,-1)	176.6432	-DE/DX = 0.0	!
! A201	L(16,15,25,3,-2)	199.0165	-DE/DX = 0.0	!





G3:M1:V1 - Gaussian Calculation Setup

Title: **CaC\_nano cage**  
Keywords: **#p opt uwb97xd/genecp pop=nbo int=ultrafine pseudo=read scf=tight**  
Charge/Mult.: **0 2**

Job Type	Method	Title	Link 0	General	Guess	Pop.	PBC	Solvation	Add. Inp.	Preview
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Multilayer ONIOM Model

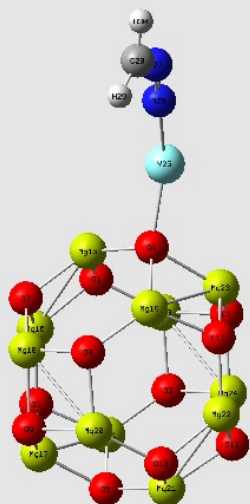
Method: Ground State | DFT... | Unrestricted | WB97XD  
Basis Set: GENECP  
Charge: 0 | Spin: Doublet

Use sparse matrices

Additional Keywords: int=ultrafine pseudo=read scf=tight

Scheme: (Unnamed Scheme)

Buttons: Submit... Quick Launch Cancel Edit... Retain Defaults



G4:M1:V1 - Gaussian Calculation Setup

Title: **CaC\_nano cage**  
Keywords: **#p opt uwb97xd/genecp pop=nbo int=ultrafine pseudo=read scf=tight**  
Charge/Mult.: **0 2**

Job Type	Method	Title	Link 0	General	Guess	Pop.	PBC	Solvation	Add. Inp.	Preview
----------	--------	-------	--------	---------	-------	------	-----	-----------	-----------	---------

```
Mg,O,C,N,H 0  
6-311+G(d,p)  
****  
Y 0  
SDD  
****  
  
Y 0  
SDD
```

Write Additional Input

Additional Keywords: int=ultrafine pseudo=read scf=tight

Scheme: (Unnamed Scheme)

Buttons: Help Update Assign to Molecule Group

**Figure 2:** Pictorial projection of the computational methods used.